Supplementary Material

to

New and extended parameterization of the thermodynamic model AIOMFAC: Calculation of activity coefficients for organic-inorganic mixtures containing carboxyl, hydroxyl, carbonyl, ether, ester, alkenyl, alkyl, and aromatic functional groups

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Complete data comparison: AIOMFAC vs. measurements

The following pages provide a graphical database overview by means of a complete set of figures, showing the experimental data and corresponding AIOMFAC calculations for all datasets used for the determination of the new main group ↔ ion interaction parameters.

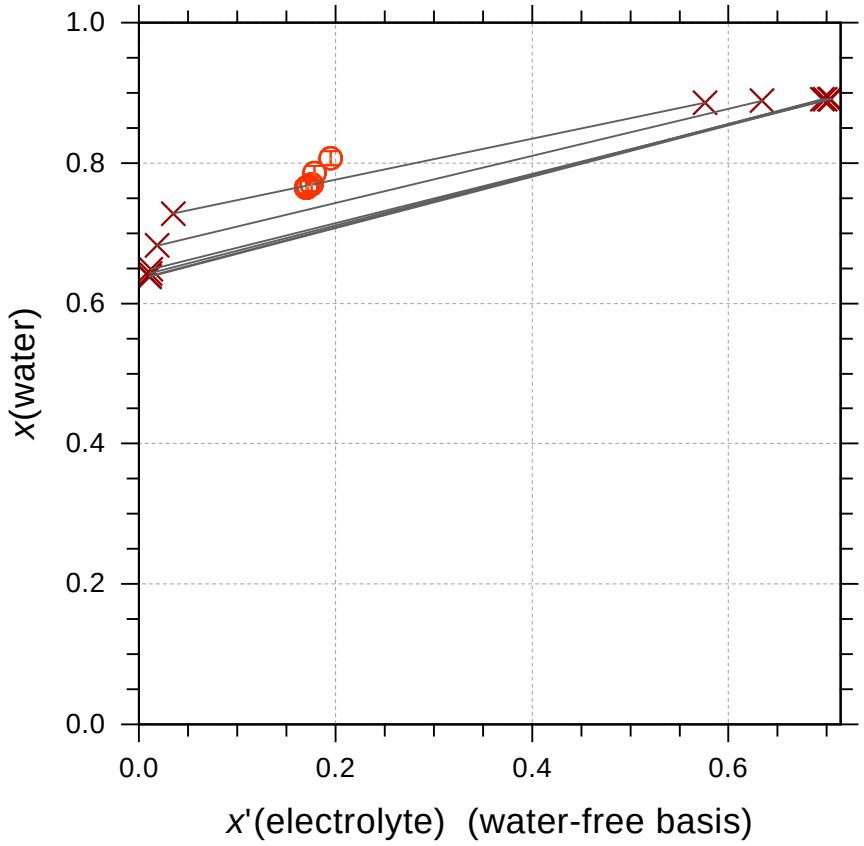
General remarks regarding the presentation of the datasets / figures:

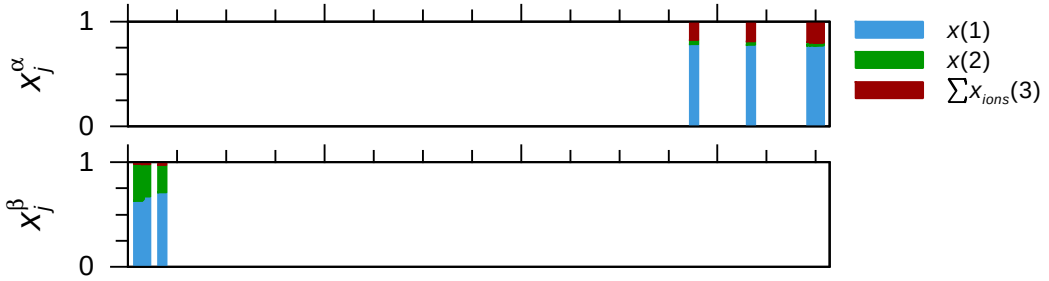
- The figures are sorted in the same sequence as the datasets are listed in Table 2 of the main article, i.e., sorted (1.) by organic compound class and (2.) inorganic electrolyte. Each figure is given a unique number, printed in the upper left corner, followed by the list of system components and the temperature range of the measurements.
- "Goodness of fit". Printed on the lower right side of each figure is a box with information regarding the initial weighting of the dataset and its overall contribution to the value of the objective function, F_{obj} (Eq. 8). This serves as a measure of the "goodness of fit" pertaining to the respective dataset (the smaller its contribution, the better), calculated with AIOMFAC based on the interaction parameters (Table 7), that have been determined with the objective of good overall model behavior regarding the ensemble of data in the database.
- SLE data. The colors of the symbols used for the presentation of solid-liquid equilibria data indicate the component, which is saturated with respect to a solid phase: red in case of an inorganic salt and green in case of a saturated organic compound.
- LLE data. In case of liquid-liquid equilibria data of ternary systems, where measured and computed phase compositions and corresponding tie-lines are shown, representations with both types of coordinate systems, as in Fig. 5 of the main article, are shown on consecutive pages. Concerning ternary mixtures where a two-phase system was found, while the phase separation computation with AIOMFAC predicts a one-phase solution, there is only one AIOMFAC symbol plotted, i.e., the initial composition of a phase separation computation (that AIOMFAC predicts to be stable), see e.g., Fig. S0001.

Fig. S0001 (AIOMFAC_output_1053)

H_2O (1) + Ethanol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K





left y-axis:

× (NH4)2SO4+Ethanol+Water_LLE_Wang

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1053) = 0.300

dataset contribution to F_{obj}:

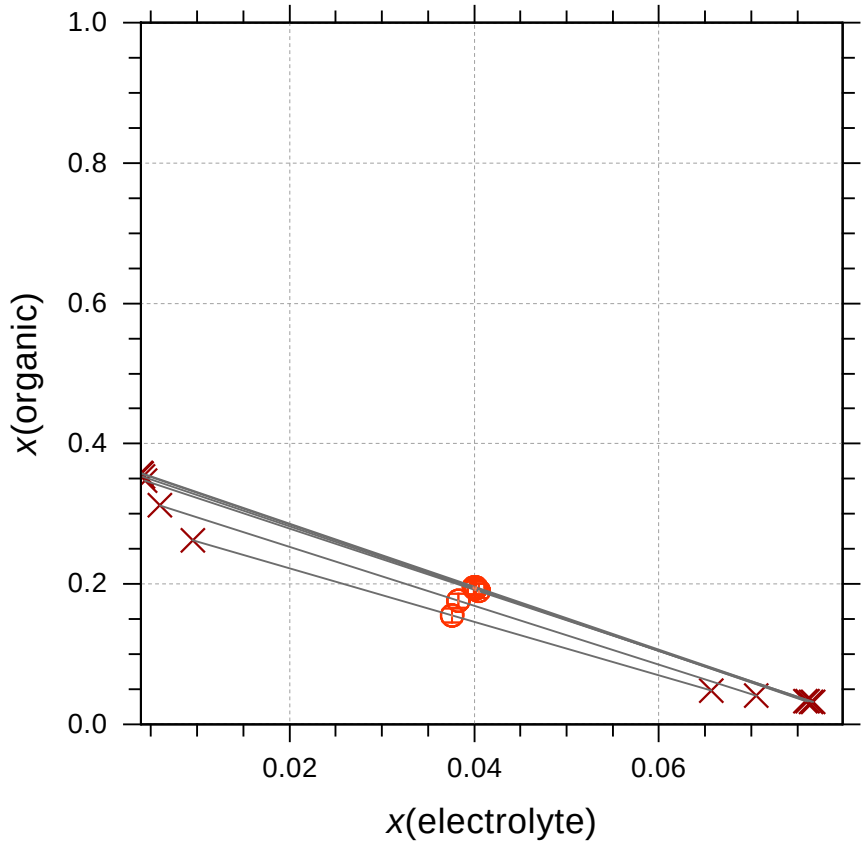
fval(1053) = 4.6248E+00

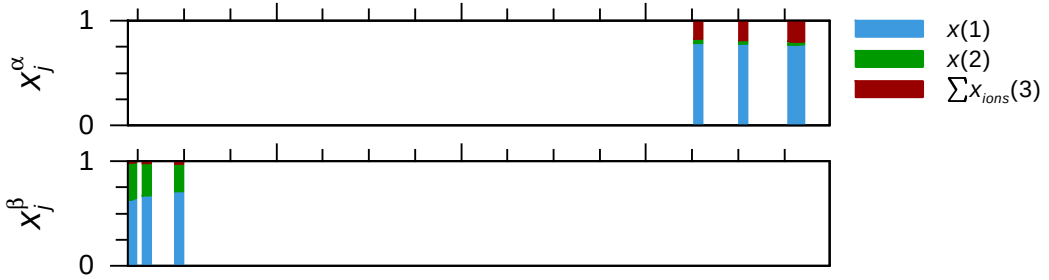
rel. contribution = 2.1993 %

Fig. S0001a (AIOMFAC_output_1053)

H_2O (1) + Ethanol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K





left y-axis:

× (NH4)2SO4+Ethanol+Water_LLE_Wang

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1053) = 0.300

dataset contribution to F_{obj}:

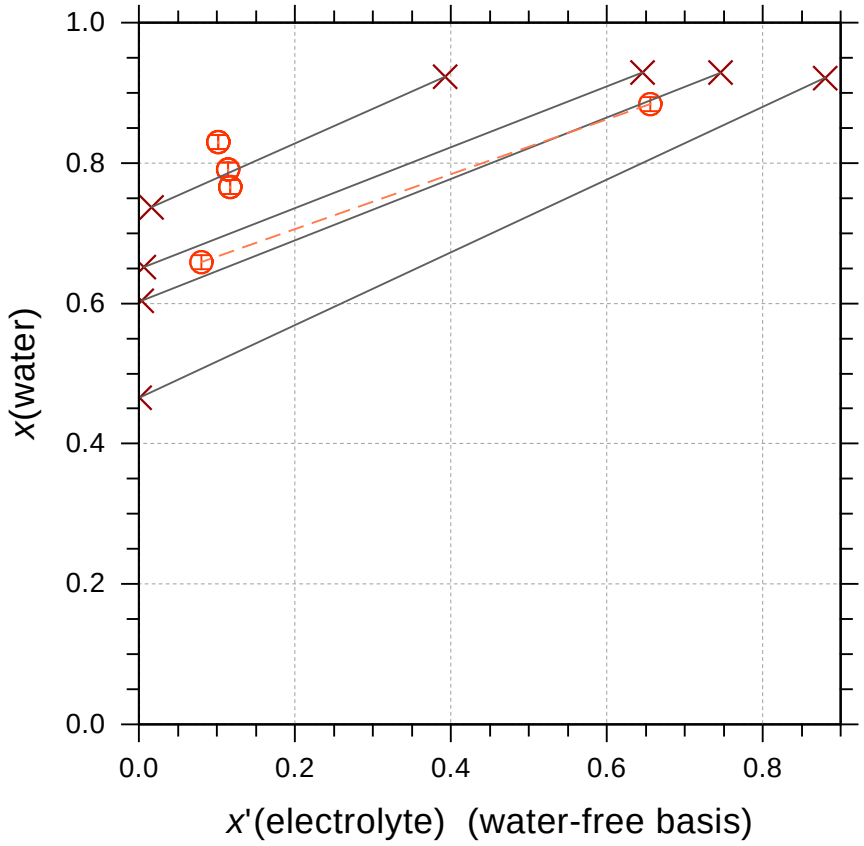
fval(1053) = 4.6248E+00

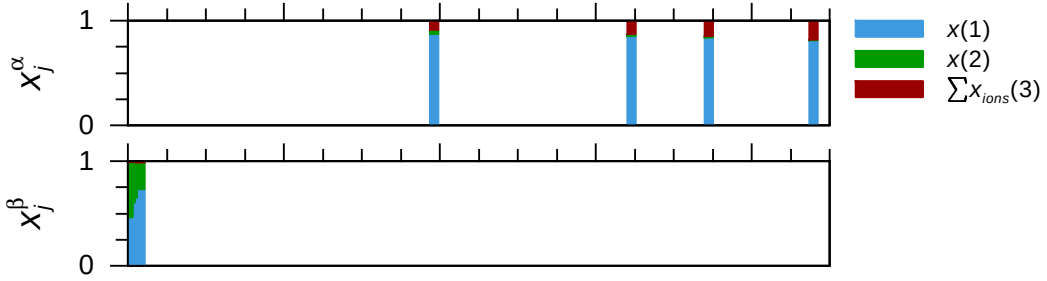
rel. contribution = 2.1993 %

Fig. S0002 (AIOMFAC_output_1063)

H_2O (1) + 2-Propanol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K





left y-axis:

× (NH4)2SO4+2-Propanol+Water_LLE_Sun

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1063) = 1.000

dataset contribution to F_{obj}:

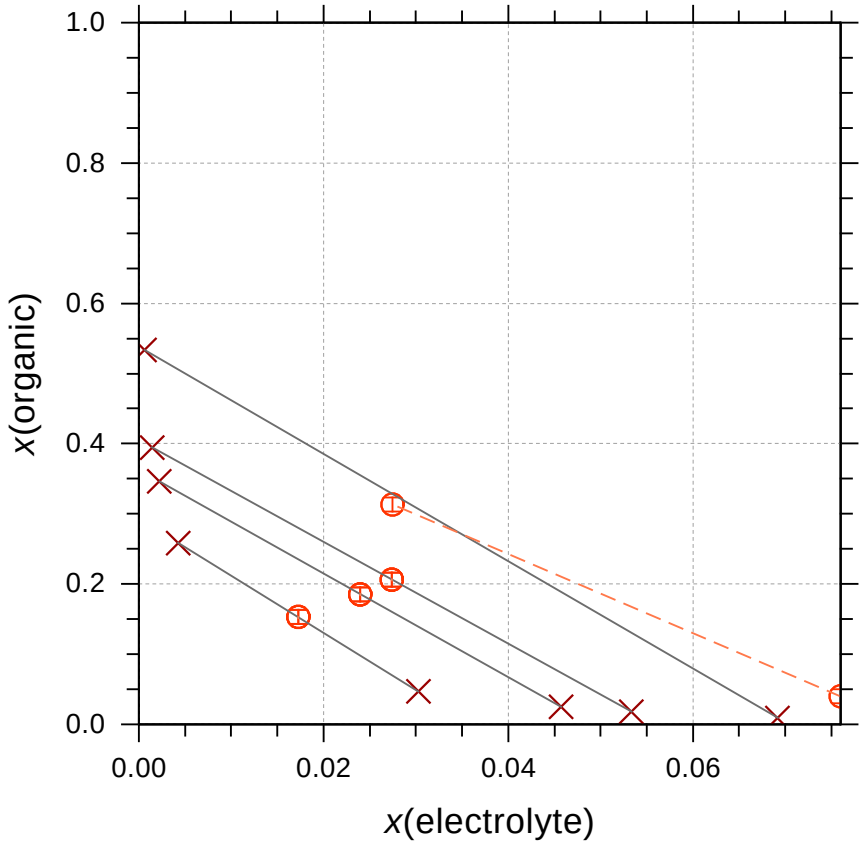
fval(1063) = 8.1480E-01

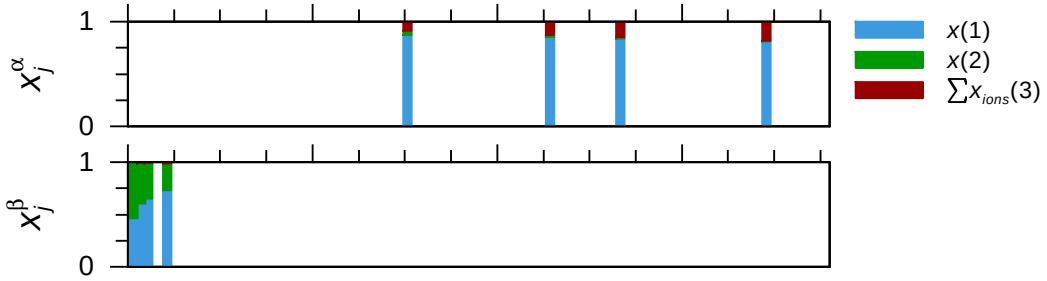
rel. contribution = 0.3875 %

Fig. S0002a (AIOMFAC_output_1063)

H_2O (1) + 2-Propanol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K





left y-axis:

× (NH4)2SO4+2-Propanol+Water_LLE_Sun

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1063) = 1.000

dataset contribution to F_{obj}:

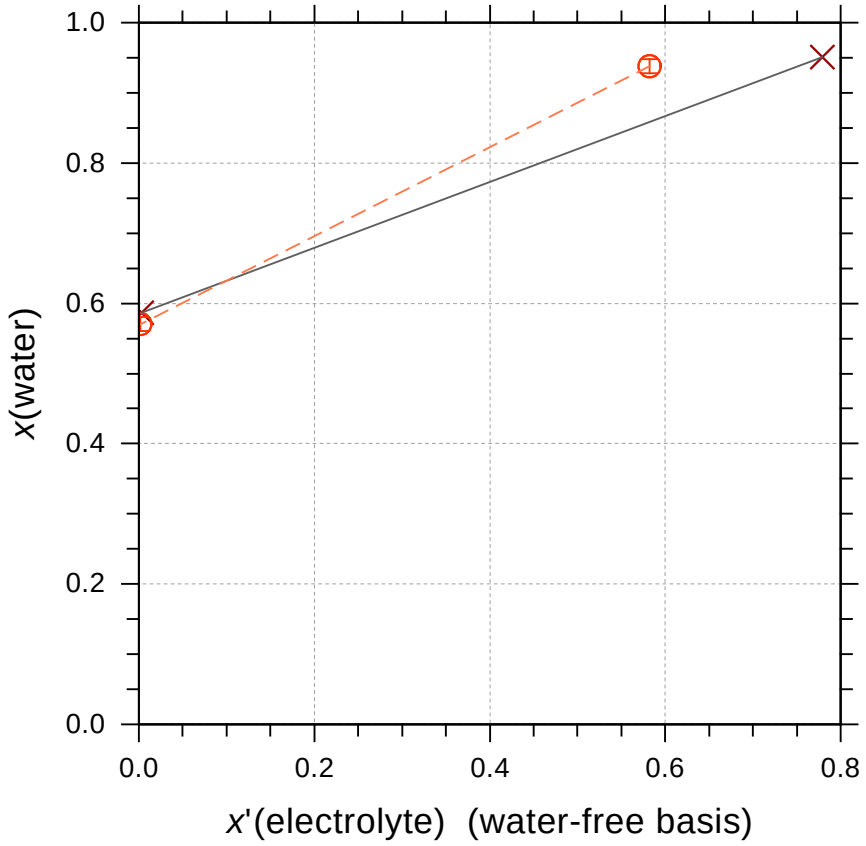
fval(1063) = 8.1480E-01

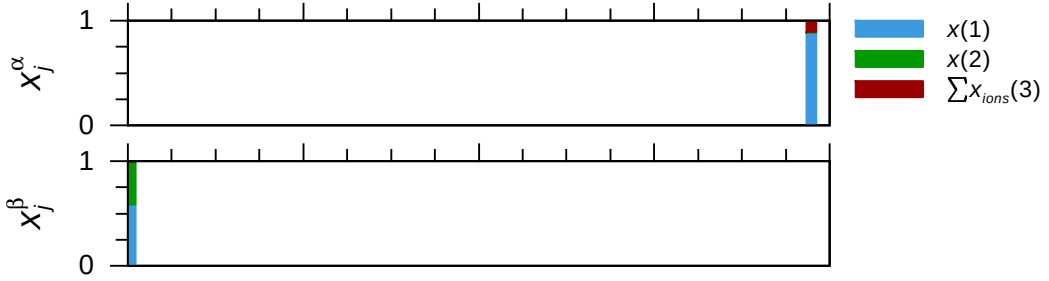
rel. contribution = 0.3875 %

Fig. S0003 (AIOMFAC_output_1055)

H_2O (1) + *tert*-Butanol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K





left y-axis:

× (NH4)2SO4+tert-Butanol+Water_LLE_Kiss

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1055) = 1.000

dataset contribution to F_{obj}:

fval(1055) = 1.1648E-01

rel. contribution = 0.0554 %

Fig. S0003a (AIOMFAC_output_1055)

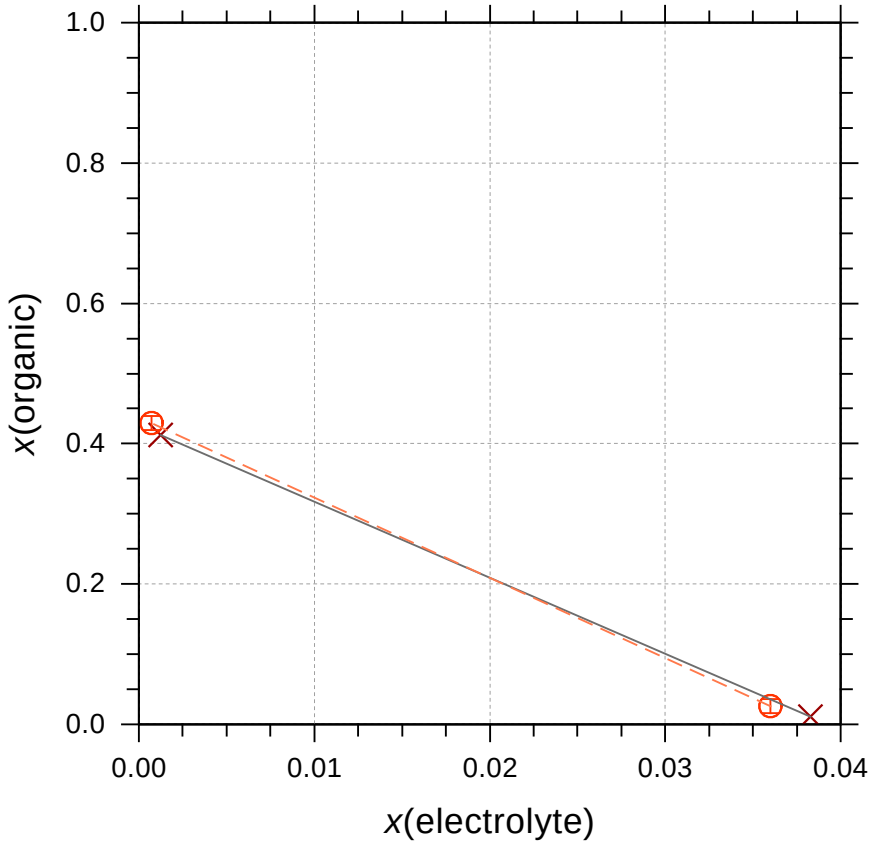
H_2O (1) + *tert*-Butanol (2) + $(NH_4)_2SO_4$ (3)

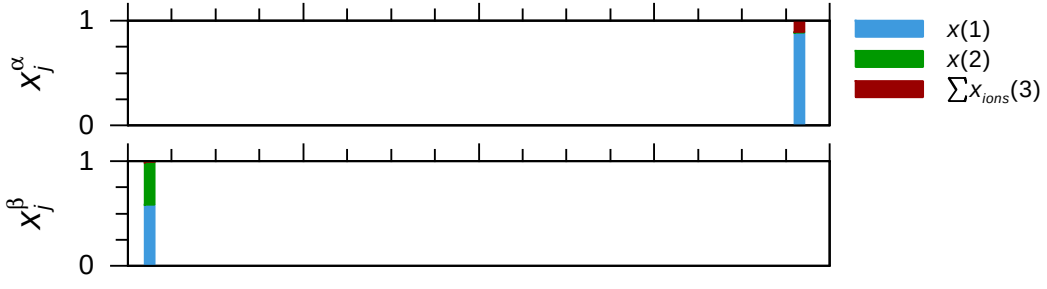
Temperature: 298 K

left y-axis:

× (NH4)2SO4+tert-Butanol+Water_LLE_Kiss

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(1055)$ = 1.000

dataset contribution to F_{obj}:

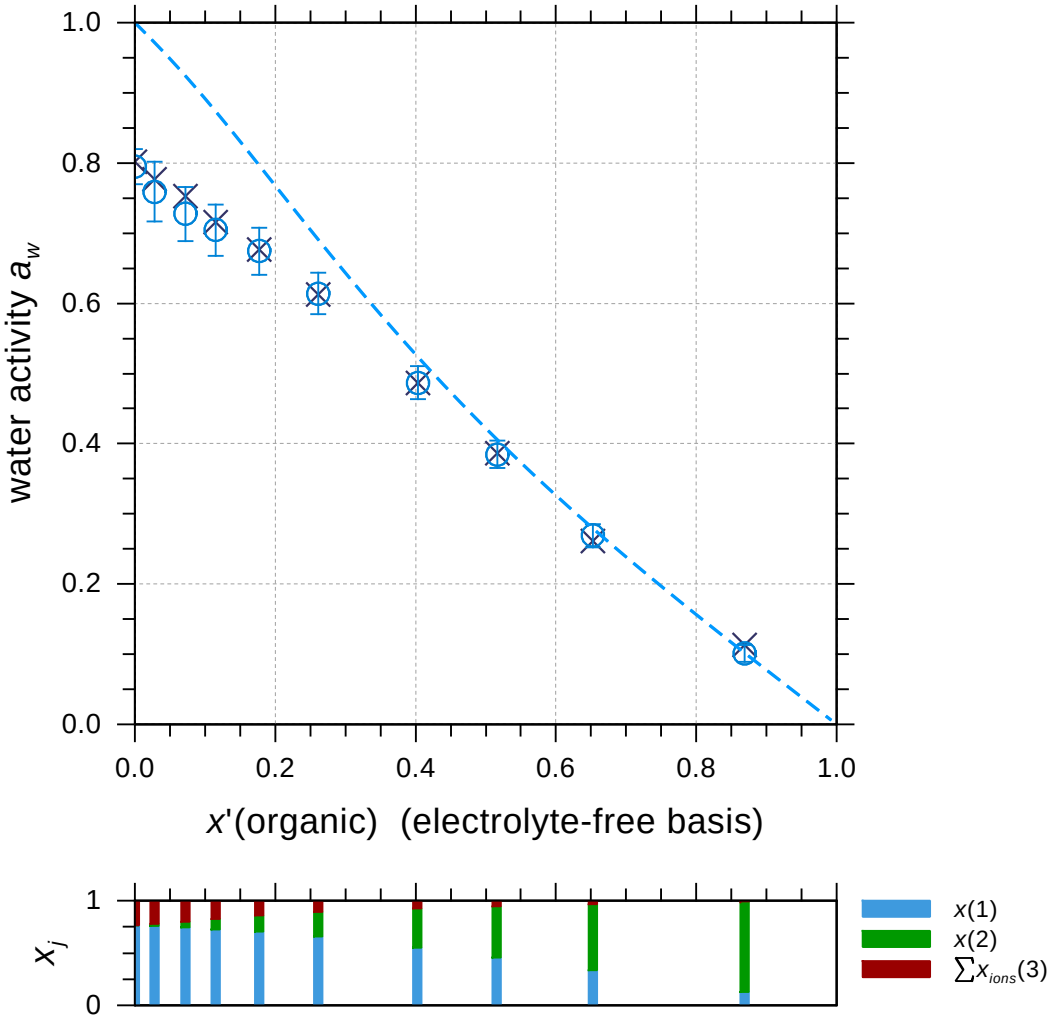
fval(1055) = 1.1648E-01

rel. contribution = 0.0554 %

Fig. S0004 (AIOMFAC_output_0091)

H_2O (1) + Glycerol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

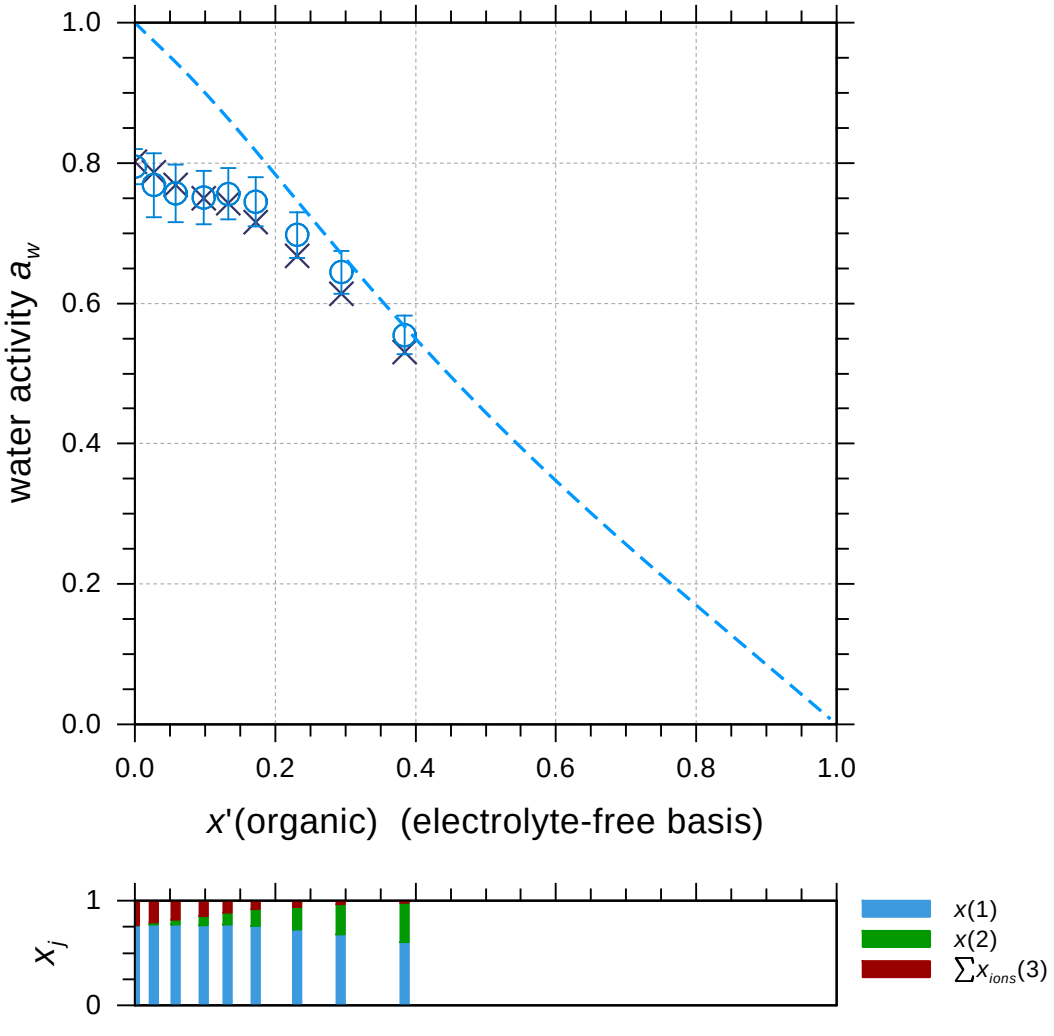


initial weighting of dataset:
$w^{init}(0091)$ = 2.000
dataset contribution to F_{obj}:
fval(0091) = 2.3980E-02
rel. contribution = 0.0114 %

Fig. S0005 (AIOMFAC_output_0092)

H_2O (1) + 1,2,4-Butanetriol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

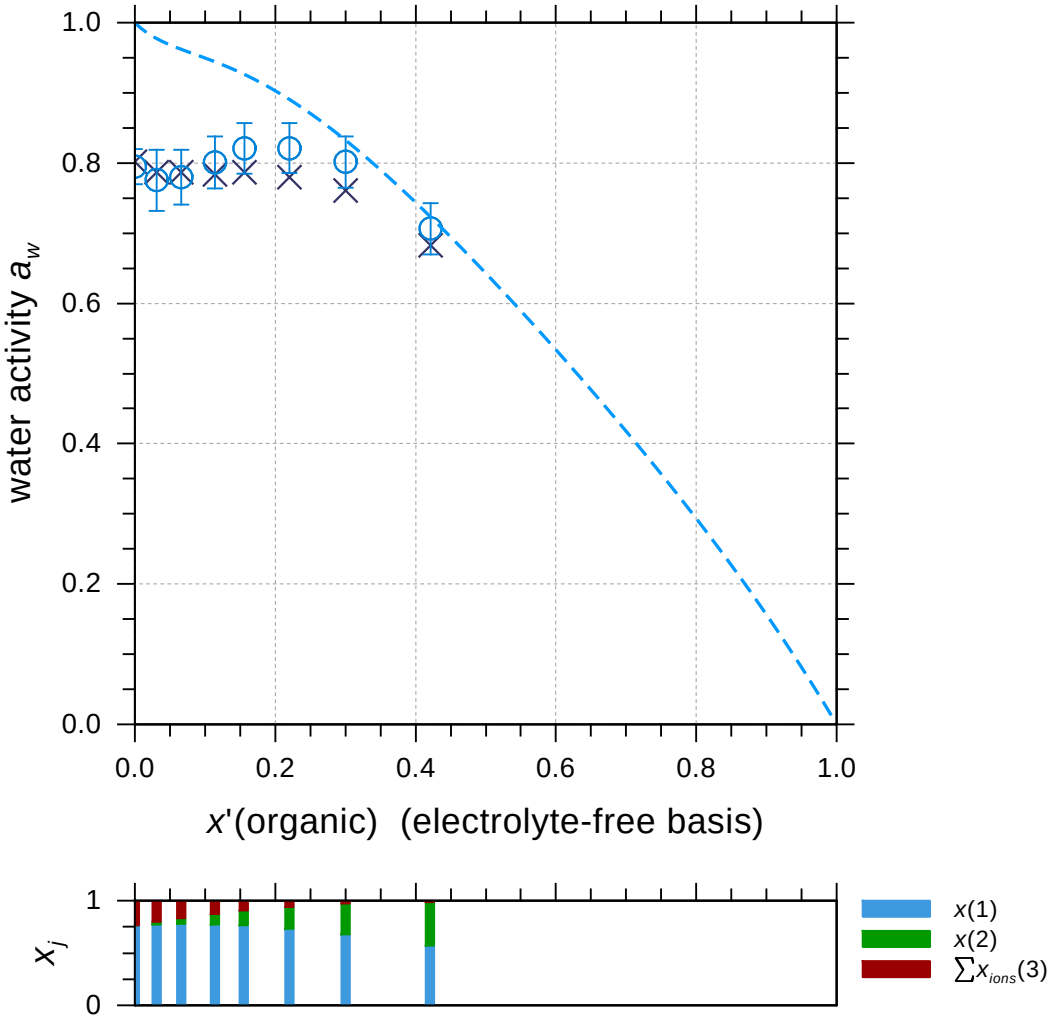


initial weighting of dataset:
$w^{init}(0092)$ = 2.000
dataset contribution to F_{obj}:
fval(0092) = 1.6714E-02
rel. contribution = 0.0079 %

Fig. S0006 (AIOMFAC_output_0093)

H_2O (1) + 1,2-Butanediol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

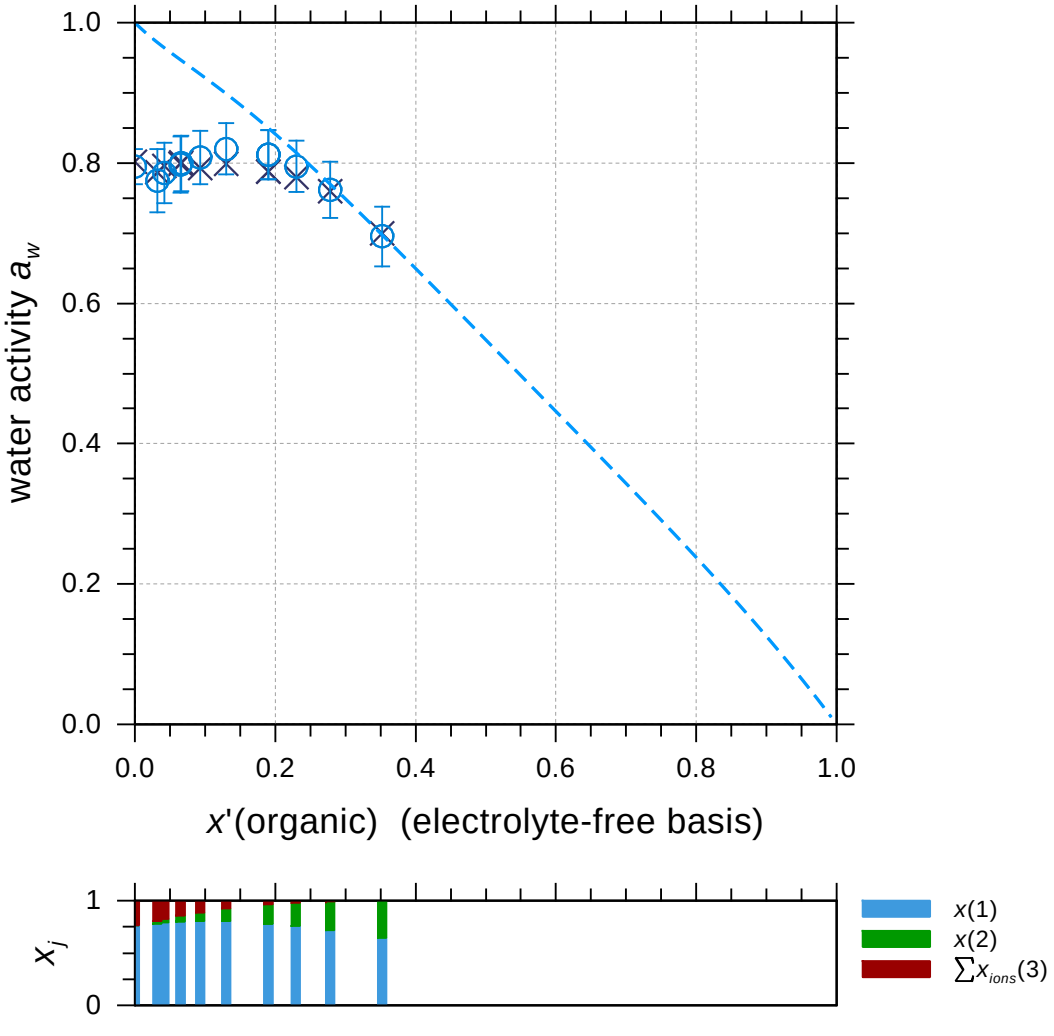


initial weighting of dataset:
$w^{init}(0093)$ = 2.000
dataset contribution to F_{obj}:
fval(0093) = 1.7328E-02
rel. contribution = 0.0082 %

Fig. S0007 (AIOMFAC_output_0094)

H_2O (1) + 1,4-Butanediol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

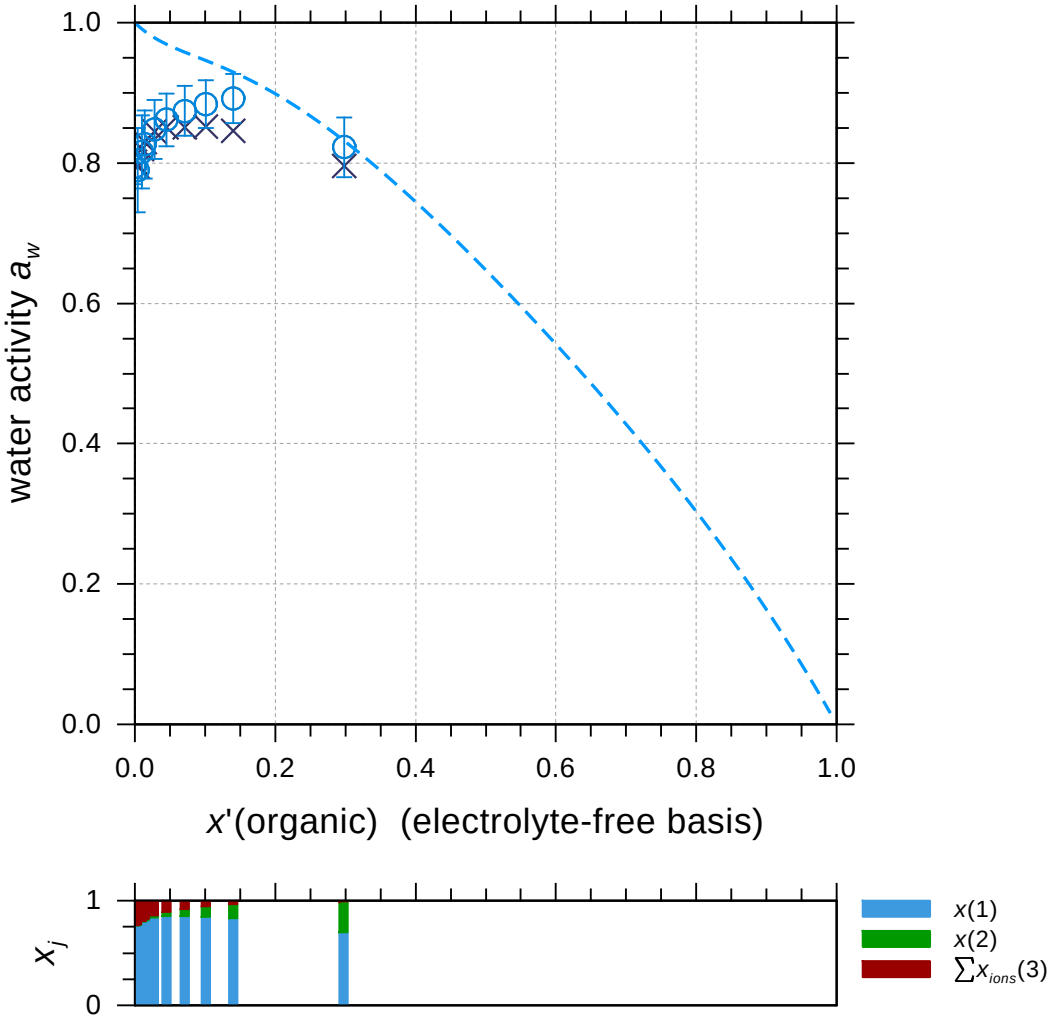


initial weighting of dataset:
$w^{init}(0094)$ = 2.000
dataset contribution to F_{obj}:
fval(0094) = 5.8265E-03
rel. contribution = 0.0028 %

Fig. S0008 (AIOMFAC_output_0095)

H_2O (1) + 2,4-Pentanediol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

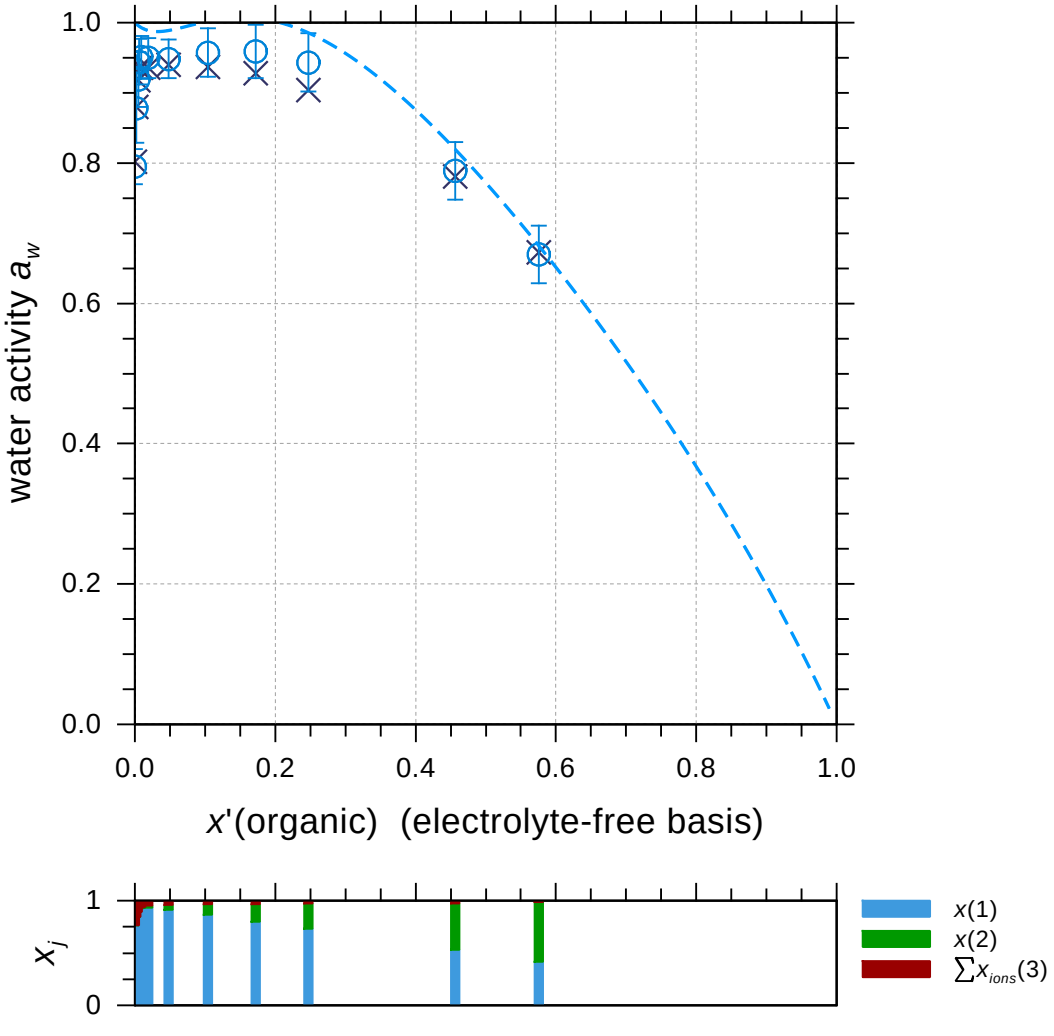


initial weighting of dataset:
$w^{init}(0095)$ = 2.000
dataset contribution to F_{obj}:
fval(0095) = 1.2028E-02
rel. contribution = 0.0057 %

Fig. S0009 (AIOMFAC_output_0096)

H_2O (1) + 1,2-Hexanediol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

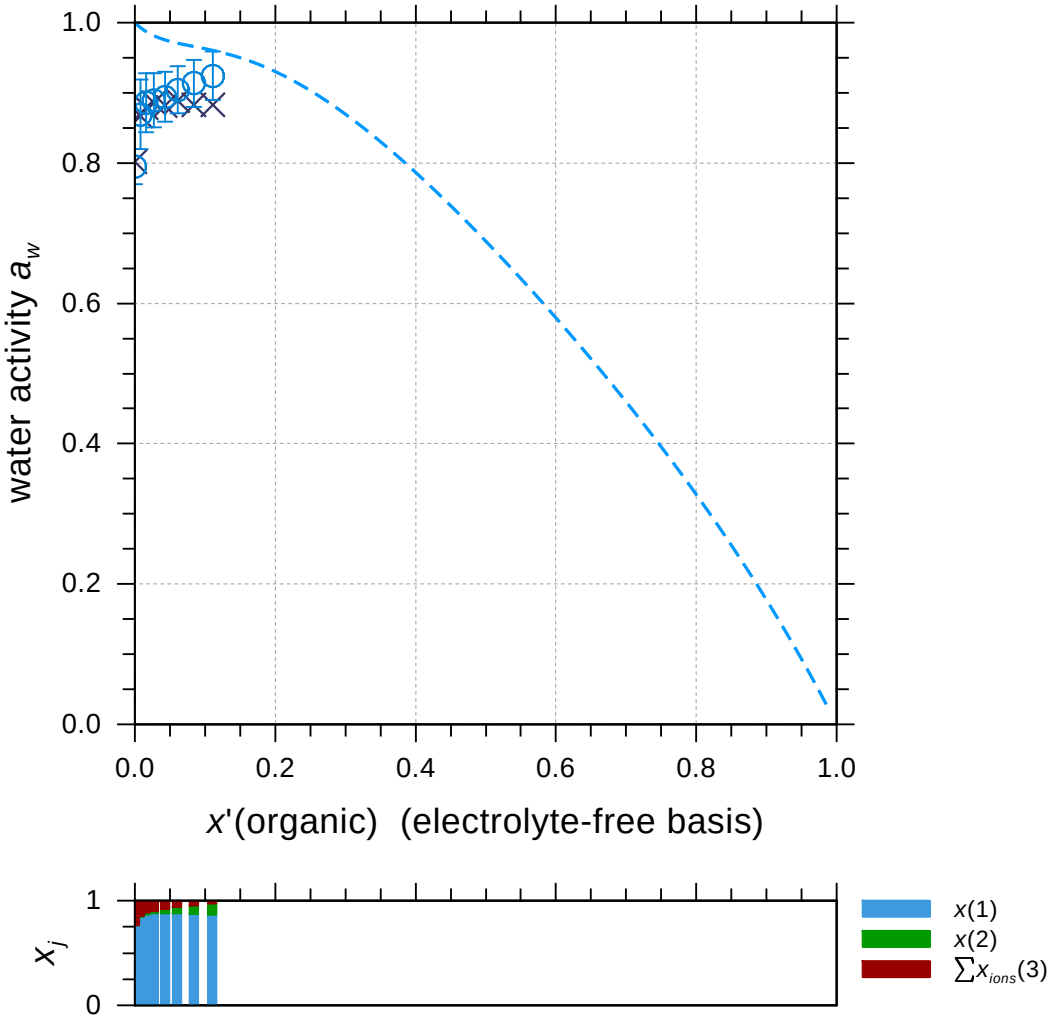


initial weighting of dataset:
$w^{init}(0096)$ = 2.000
dataset contribution to F_{obj}:
fval(0096) = 6.6671E-03
rel. contribution = 0.0032 %

Fig. S0010 (AIOMFAC_output_0097)

H_2O (1) + 2,5-Hexanediol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

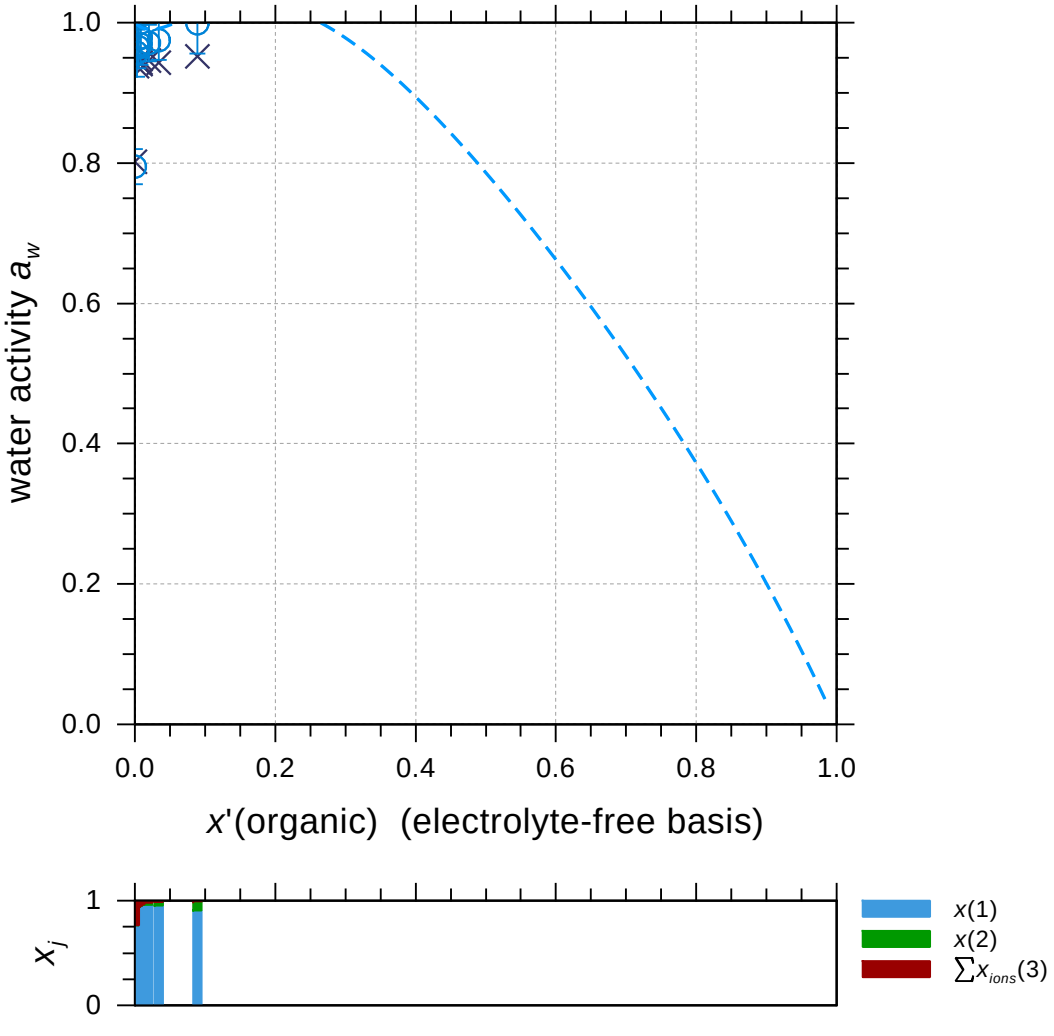


initial weighting of dataset:
$w^{init}(0097)$ = 2.000
dataset contribution to F_{obj}:
fval(0097) = 7.4965E-03
rel. contribution = 0.0036 %

Fig. S0011 (AIOMFAC_output_0098)

H_2O (1) + 1,7-Heptanediol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

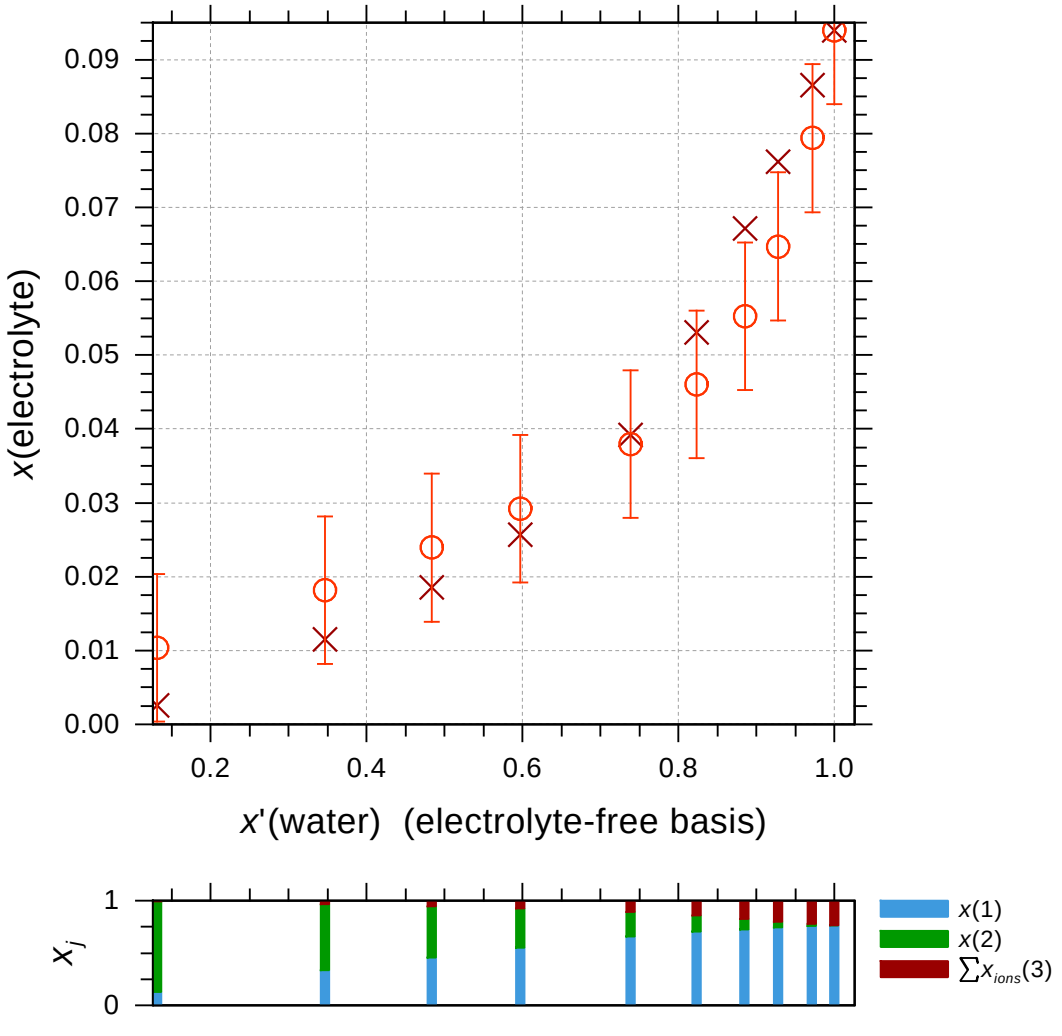


initial weighting of dataset:
$w^{init}(0098)$ = 2.000
dataset contribution to F_{obj}:
fval(0098) = 1.5829E-02
rel. contribution = 0.0075 %

Fig. S0012 (AIOMFAC_output_0949)

H_2O (1) + Glycerol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

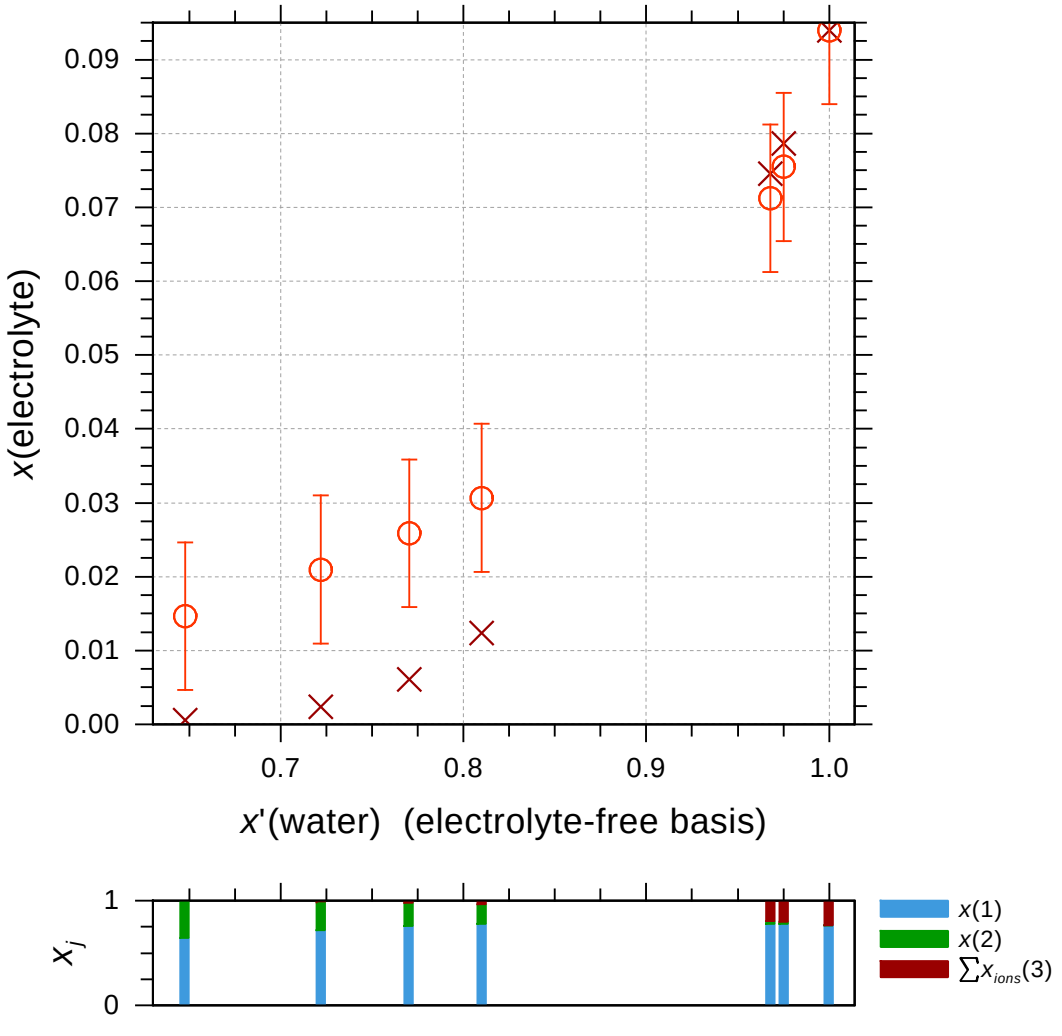


initial weighting of dataset:
w^{init}(0949) = 1.000
dataset contribution to F_{obj}:
fval(0949) = 5.8936E-01
rel. contribution = 0.2803 %

Fig. S0013 (AIOMFAC_output_0950)

H_2O (1) + 1,4-Butanediol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

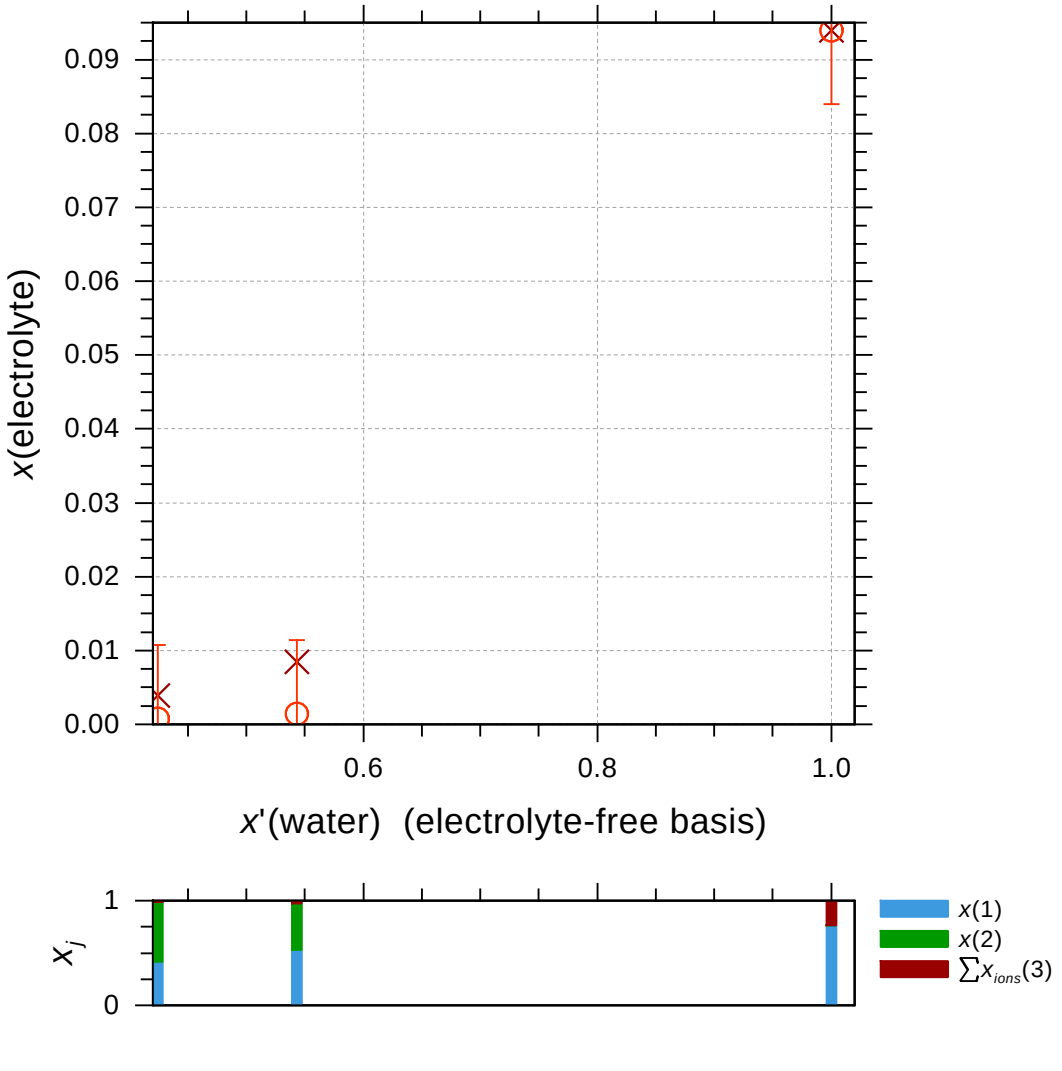


initial weighting of dataset:
$w^{init}(0950)$ = 1.000
dataset contribution to F_{obj}:
fval(0950) = 6.2258E+00
rel. contribution = 2.9606 %

Fig. S0014 (AIOMFAC_output_0951)

H_2O (1) + 1,2-Hexanediol (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

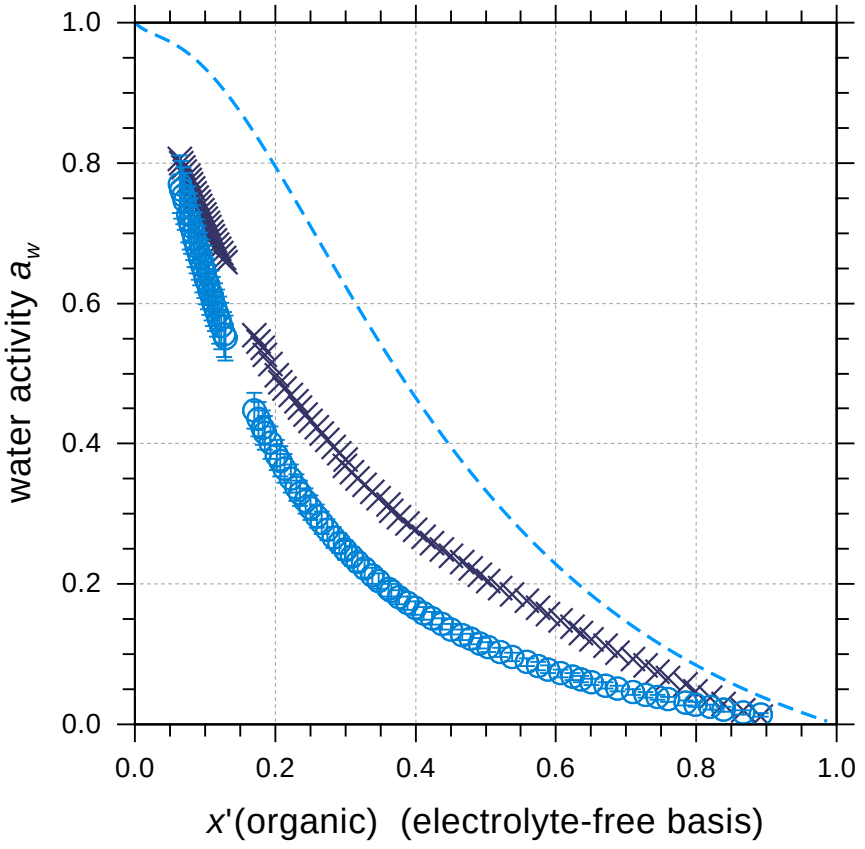


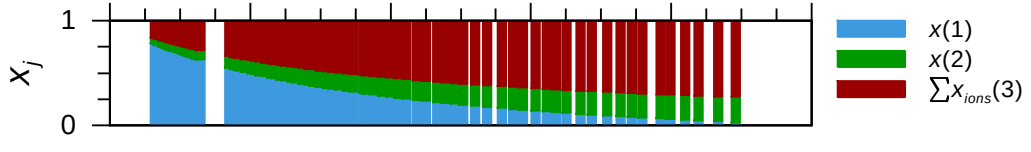
initial weighting of dataset:
$w^{init}(0951)$ = 1.000
dataset contribution to F_{obj}:
fval(0951) = 1.9717E-01
rel. contribution = 0.0938 %

Fig. S0015 (AIOMFAC_output_1039)

H_2O (1) + Levoglucosan (2) + $(NH_4)_2SO_4$ (3)

Temperature: 291 K





left y-axis:

× (NH4)2SO4+Levoglucosan+Water_EDB-aw_Lienhard

○ AIOMFAC water activity a_w

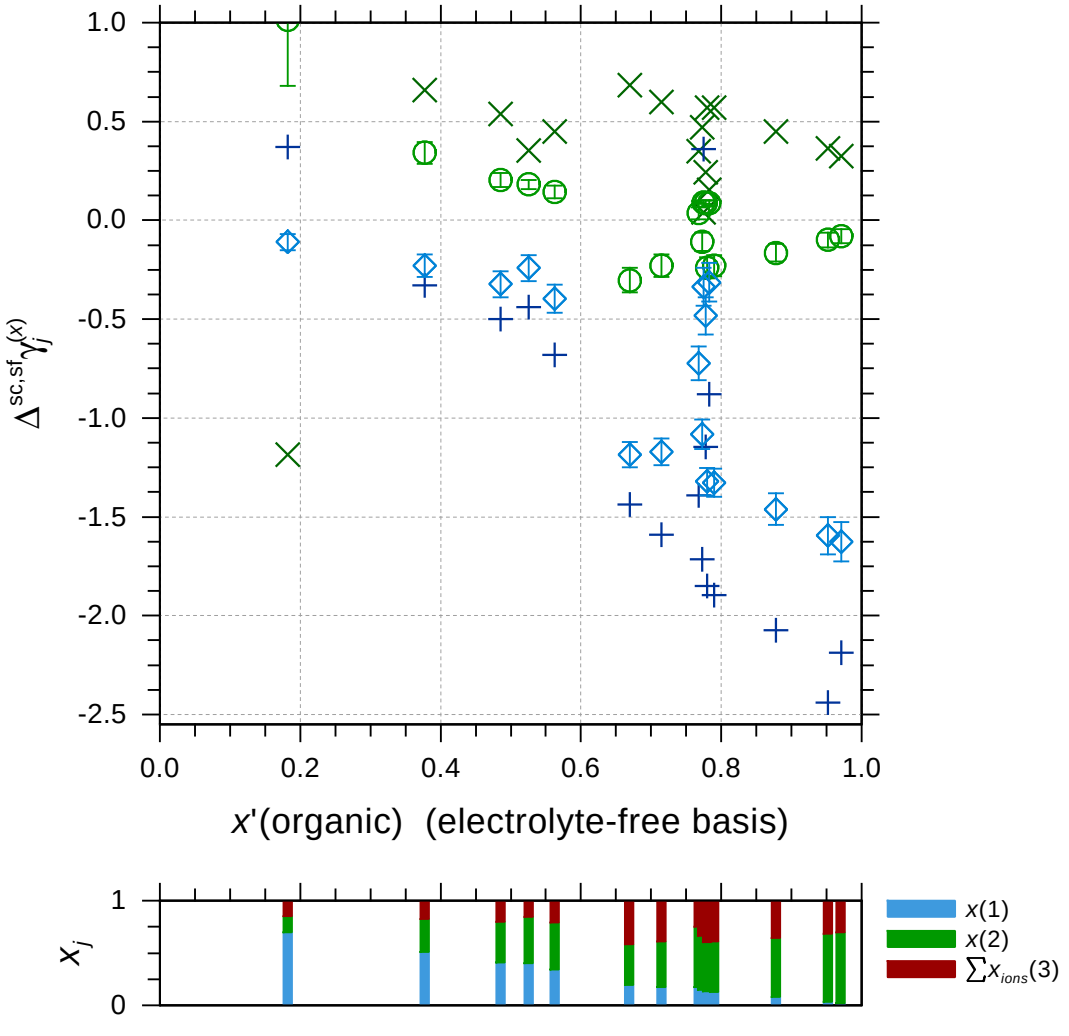
– – AIOMFAC electrolyte-free solution a_w

initial weighting of dataset:
$w^{init}(1039)$ = 1.000
dataset contribution to F_{obj}:
fval(1039) = 9.9040E-01
rel. contribution = 0.4710 %

Fig. S0016 (AIOMFAC_output_0075)

H_2O (1) + 1-Propanol (2) + $Ca(NO_3)_2$ (3)

Temperature range: 362 -- 373 K



initial weighting of dataset:

$w^{init}(0075)$ = 0.050

dataset contribution to F_{obj}:

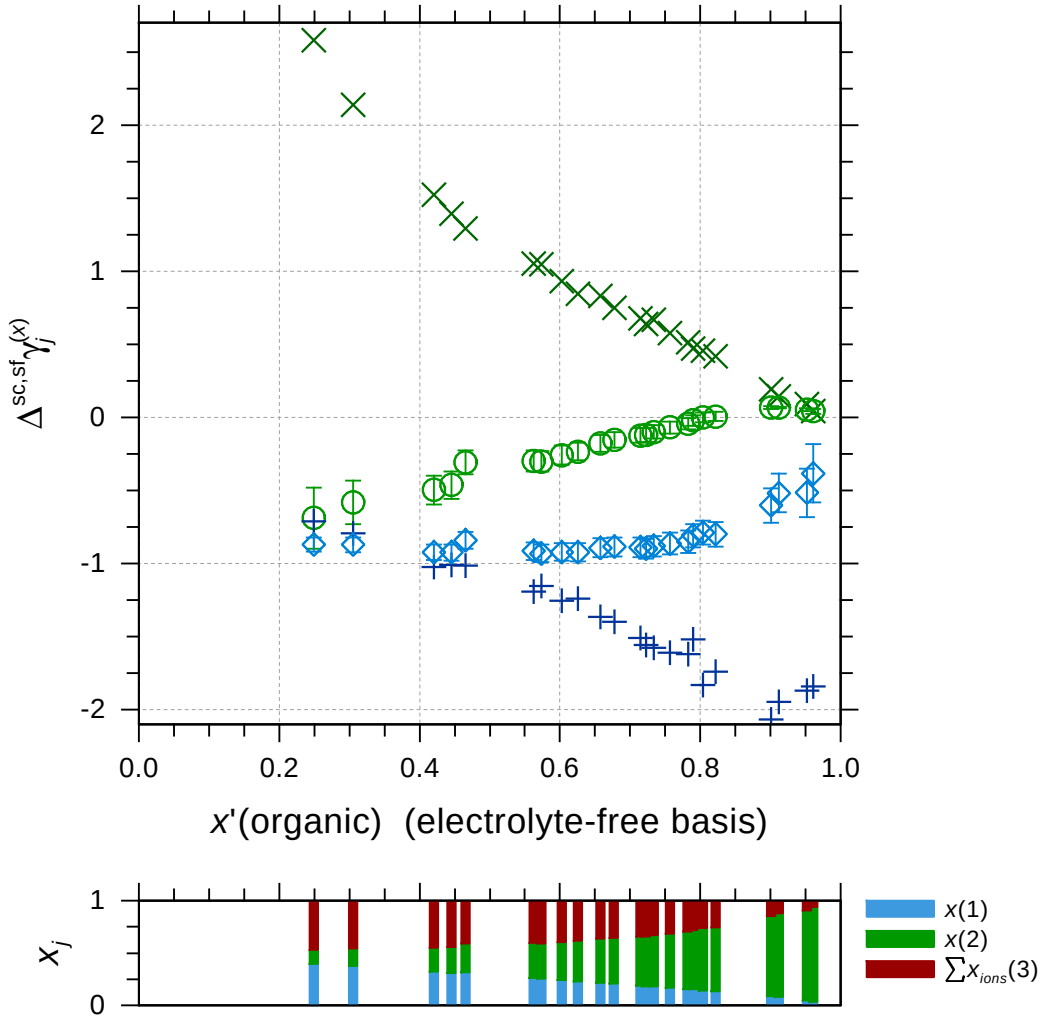
fval(0075) = 1.0215E-01

rel. contribution = 0.0486 %

Fig. S0017 (AIOMFAC_output_0076)

H_2O (1) + 2-Propanol (2) + $Ca(NO_3)_2$ (3)

Temperature range: 354 -- 361 K



initial weighting of dataset:

$w^{init}(0076)$ = 0.050

dataset contribution to F_{obj}:

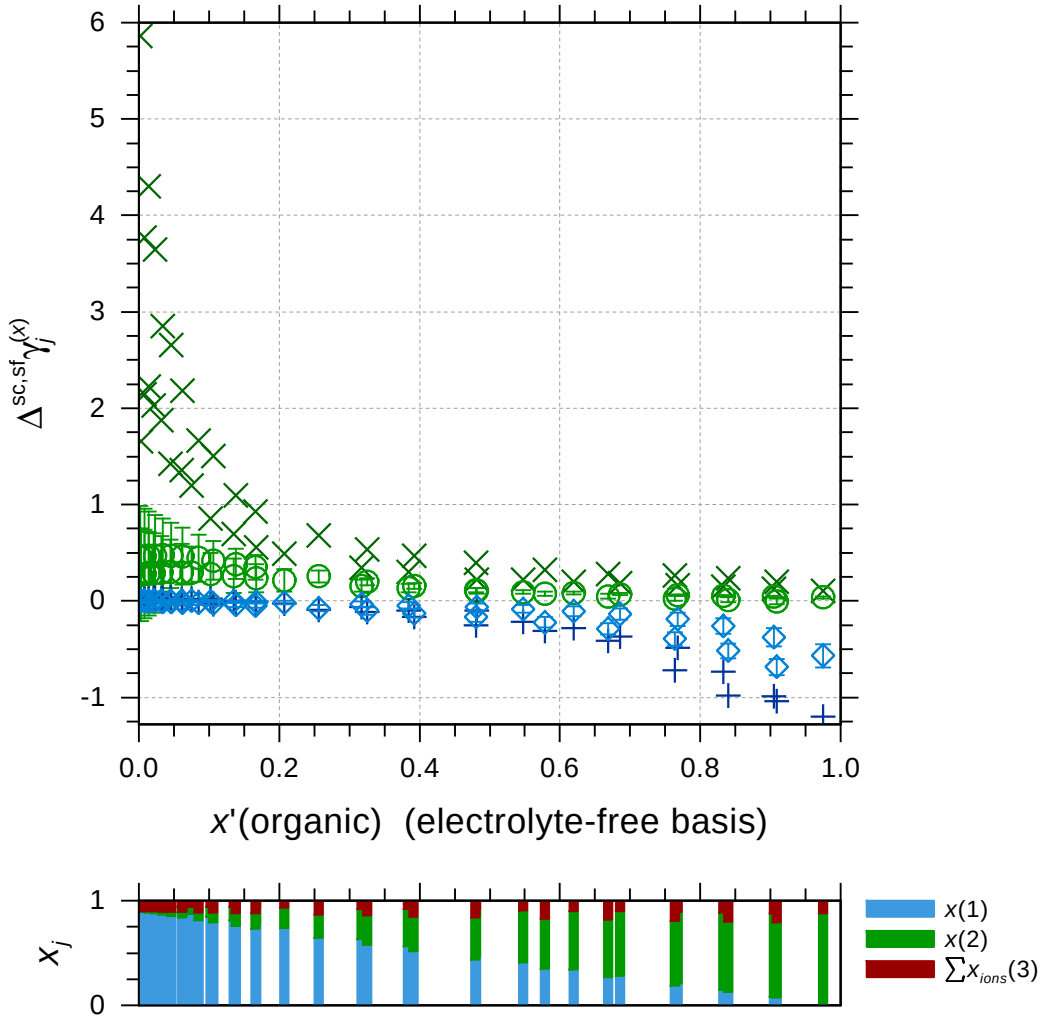
fval(0076) = 1.7274E-01

rel. contribution = 0.0821 %

Fig. S0018 (AIOMFAC_output_0077)

H_2O (1) + Ethanol (2) + $Ca(NO_3)_2$ (3)

Temperature range: 336 -- 356 K



initial weighting of dataset:

w^{init}(0077) = 0.500

dataset contribution to F_{obj}:

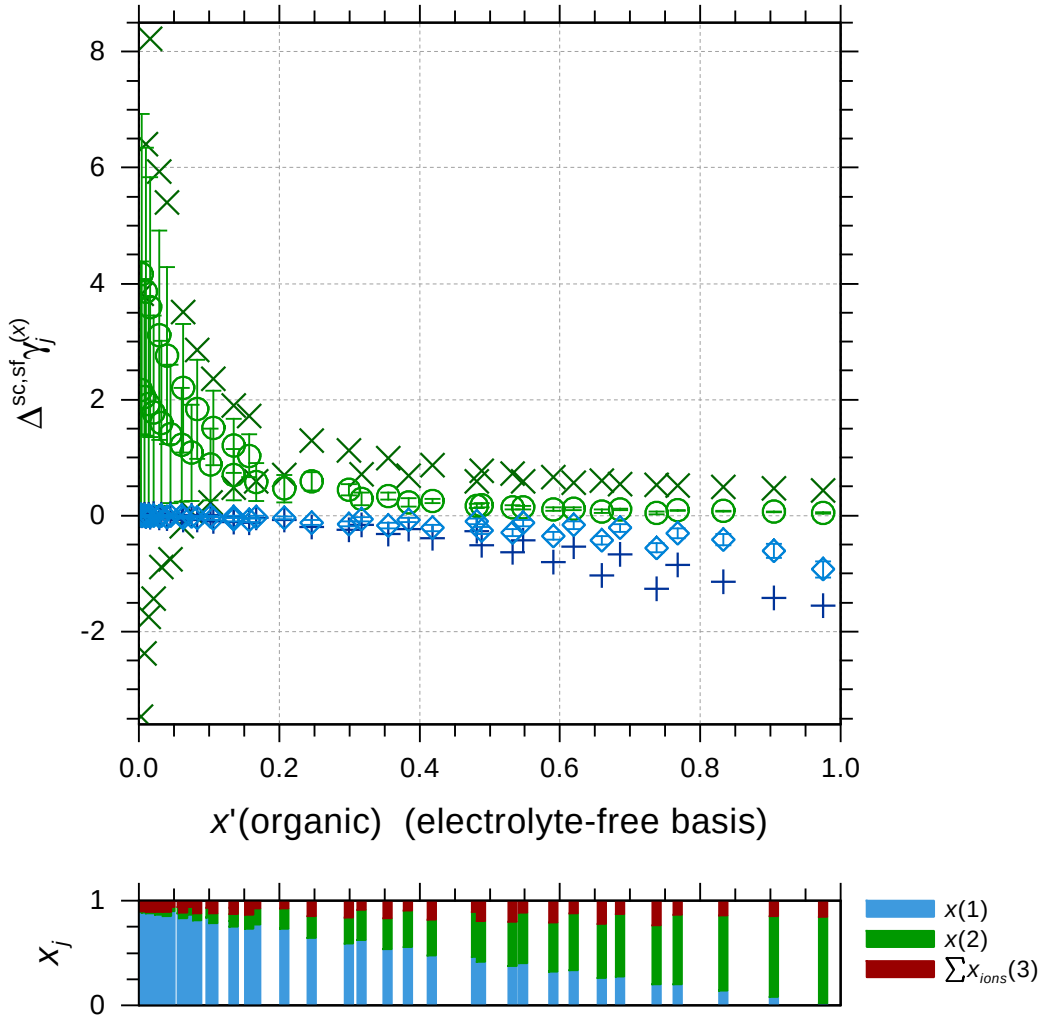
fval(0077) = 7.0766E-01

rel. contribution = 0.3365 %

Fig. S0019 (AIOMFAC_output_0078)

H_2O (1) + 2-Propanol (2) + $Ca(NO_3)_2$ (3)

Temperature range: 336 -- 355 K

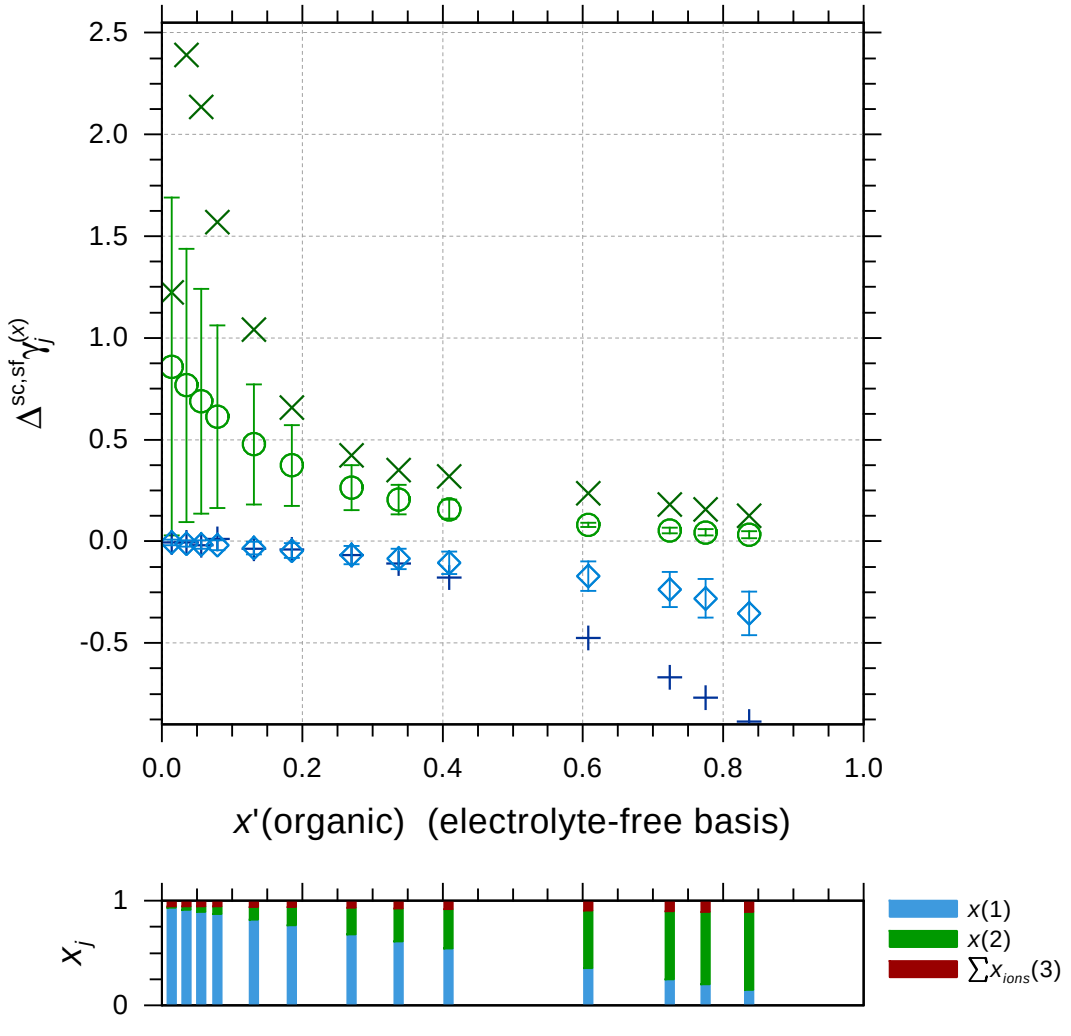


initial weighting of dataset:
$w^{init}(0078)$ = 0.500
dataset contribution to F_{obj}:
fval(0078) = 9.5257E-01
rel. contribution = 0.4530 %

Fig. S0020 (AIOMFAC_output_0063)

H_2O (1) + Ethanol (2) + $CaCl_2$ (3)

Temperature range: 308 -- 321 K



initial weighting of dataset:

w^{init}(0063) = 0.500

dataset contribution to F_{obj}:

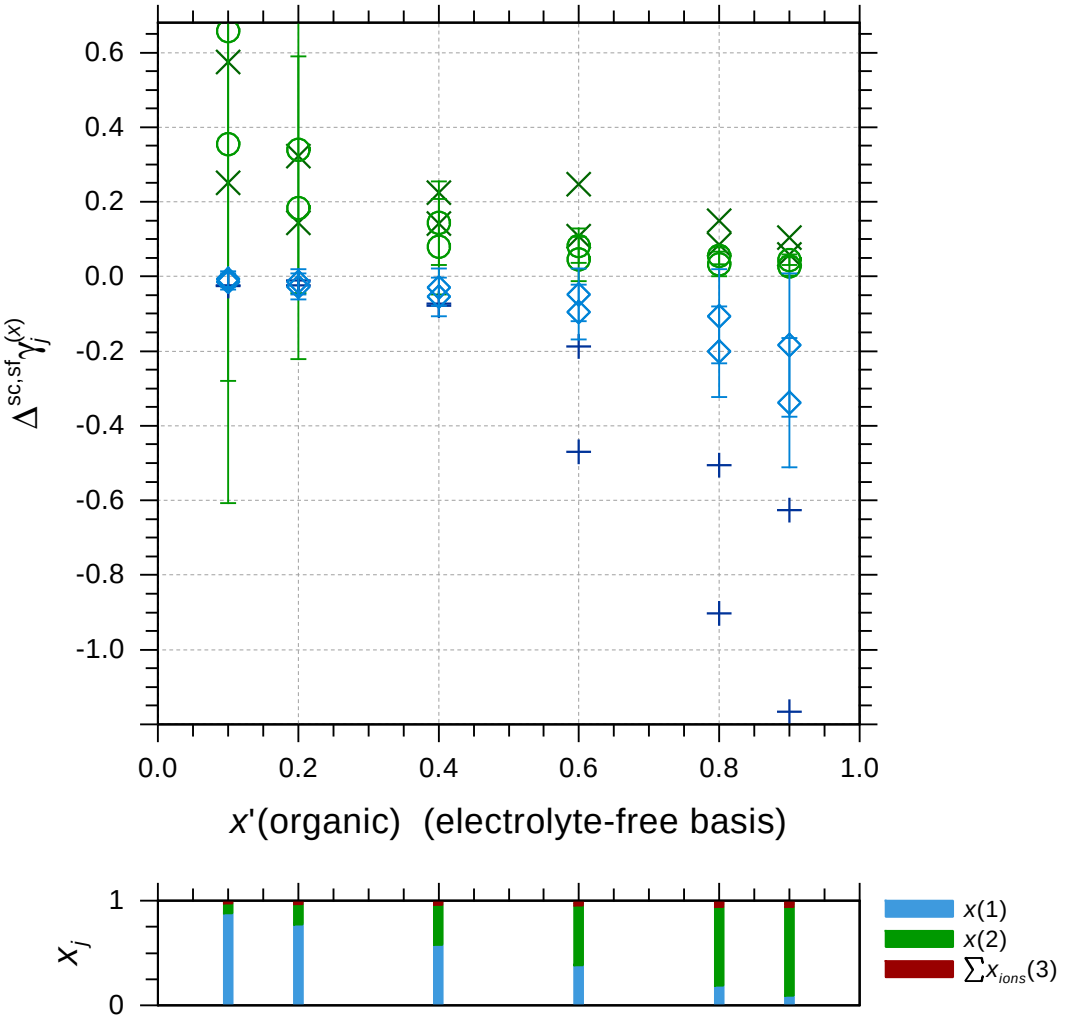
fval(0063) = 3.1988E-01

rel. contribution = 0.1521 %

Fig. S0021 (AIOMFAC_output_0064)

H_2O (1) + 2-Propanol (2) + $CaCl_2$ (3)

Temperature range: 354 -- 357 K



initial weighting of dataset:

$w^{init}(0064)$ = 0.500

dataset contribution to F_{obj}:

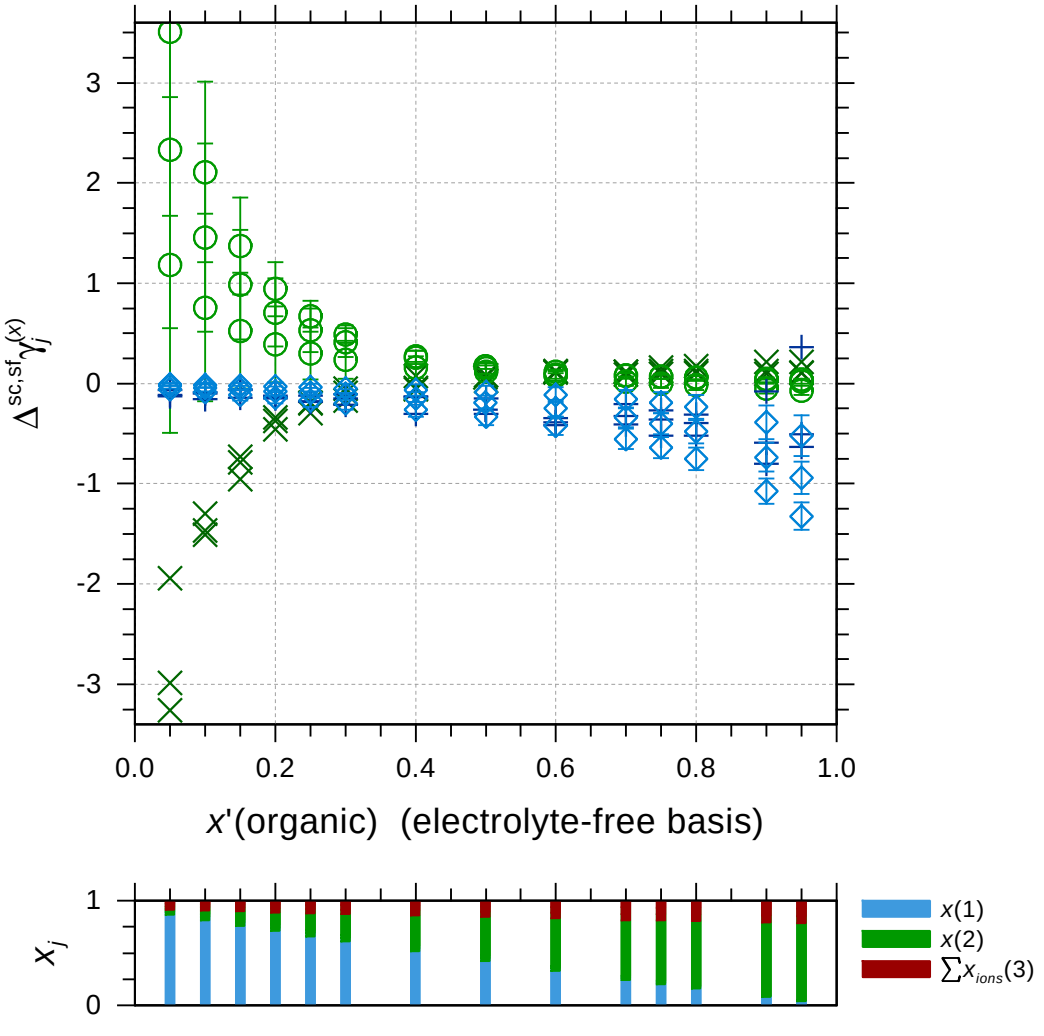
fval(0064) = 1.9963E-01

rel. contribution = 0.0949 %

Fig. S0022 (AIOMFAC_output_0065)

H_2O (1) + 2-Propanol (2) + $CaCl_2$ (3)

Temperature range: 354 -- 368 K

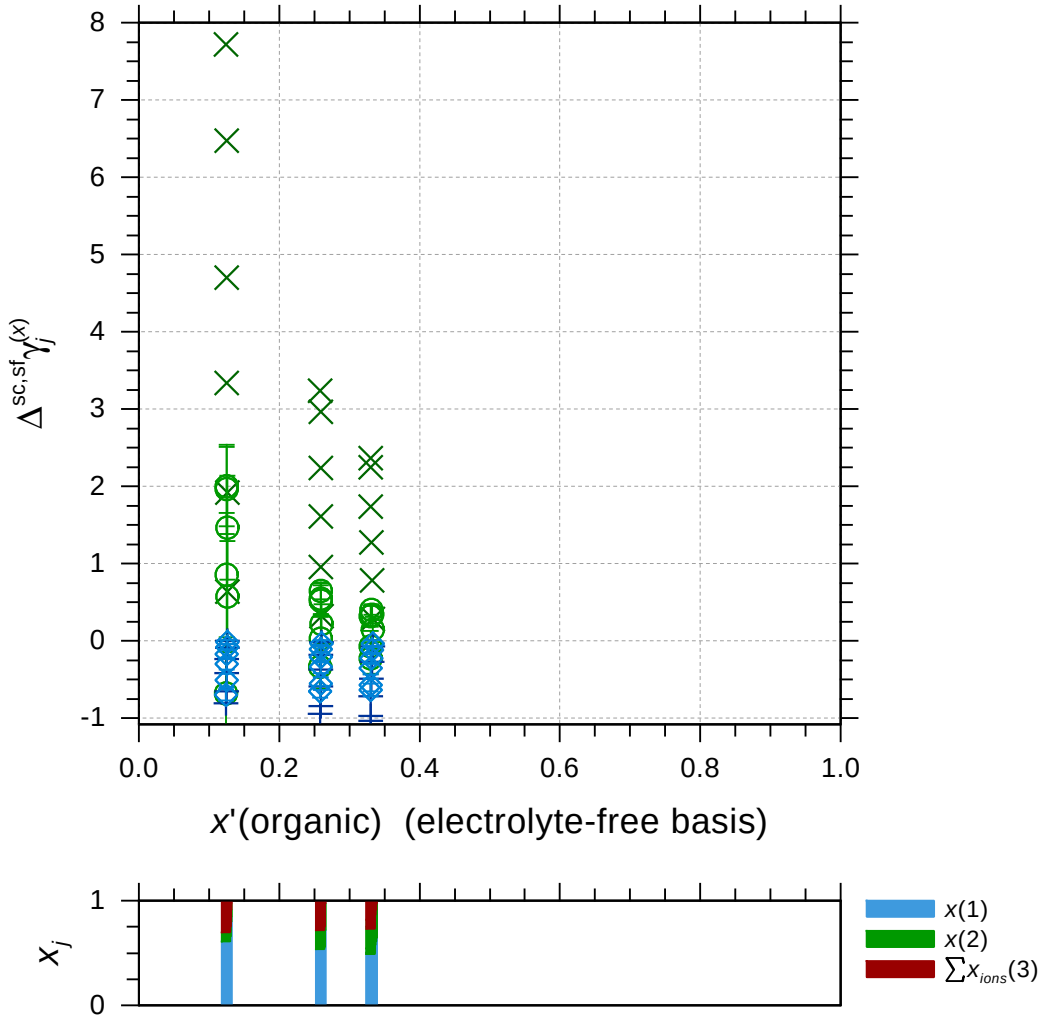


initial weighting of dataset:
$w^{init}(0065)$ = 0.000
dataset contribution to F_{obj}:
fval(0065) = 0.0000E+00
rel. contribution = 0.0000 %

Fig. S0023 (AIOMFAC_output_0066)

H_2O (1) + 2-Propanol (2) + $CaCl_2$ (3)

Temperature: 348 K

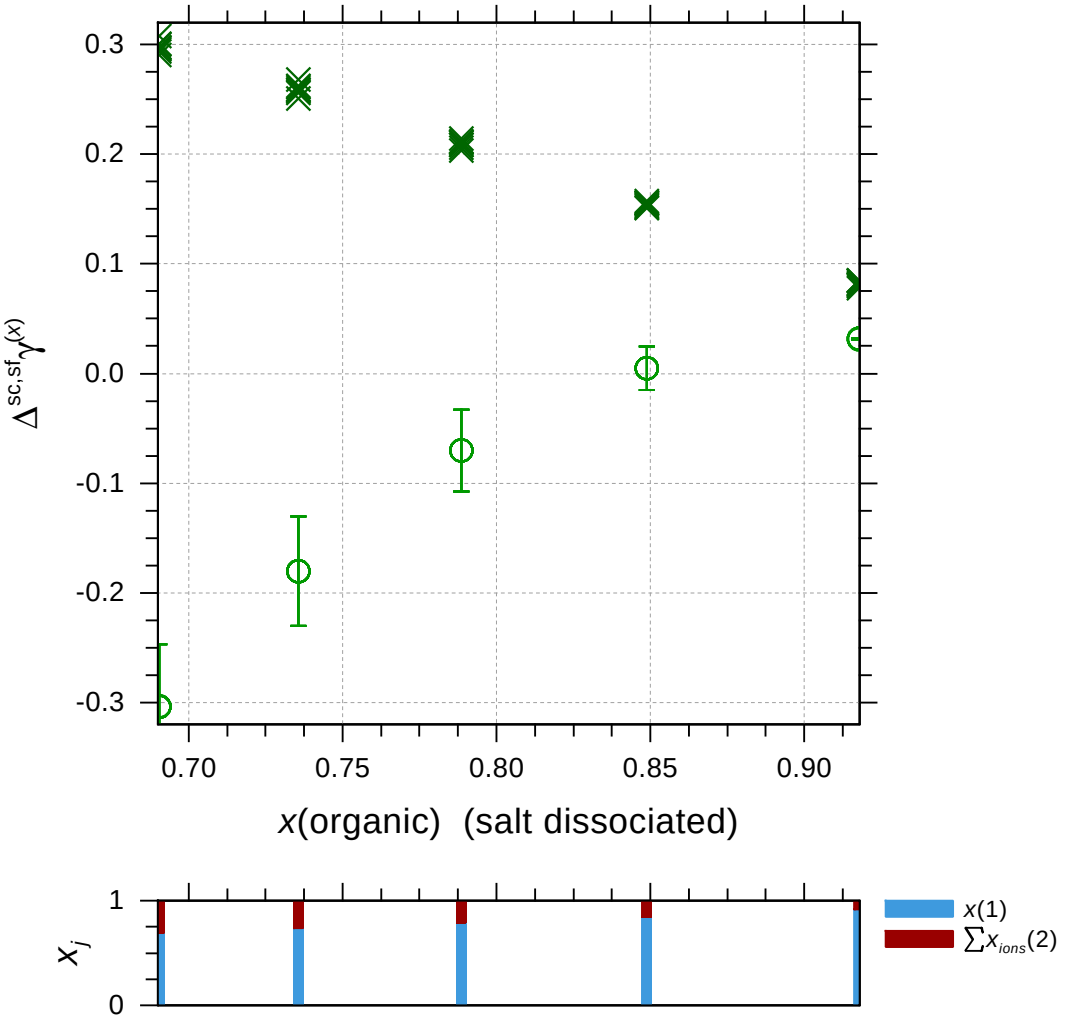


initial weighting of dataset:
w^{init}(0066) = 0.500
dataset contribution to F_{obj}:
fval(0066) = 1.3166E+00
rel. contribution = 0.6261 %

Fig. S0024 (AIOMFAC_output_0999)

1-Propanol (1) + $CaCl_2$ (2)

Temperature range: 361 -- 373 K

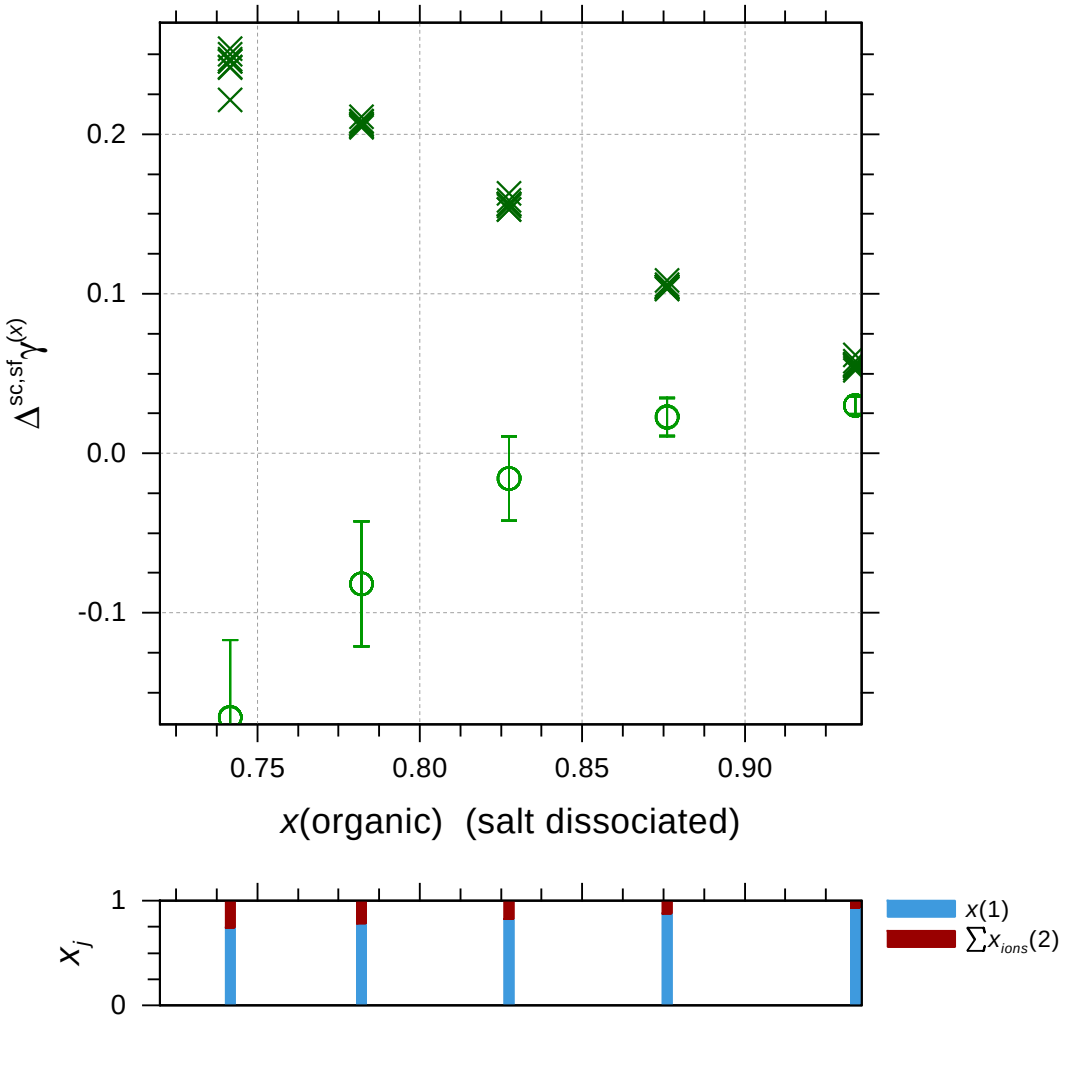


initial weighting of dataset:
$w^{init}(0999)$ = 0.010
dataset contribution to F_{obj}:
fval(0999) = 7.5730E-03
rel. contribution = 0.0036 %

Fig. S0025 (AIOMFAC_output_1000)

2-Propanol (1) + $CaCl_2$ (2)

Temperature range: 347 -- 357 K

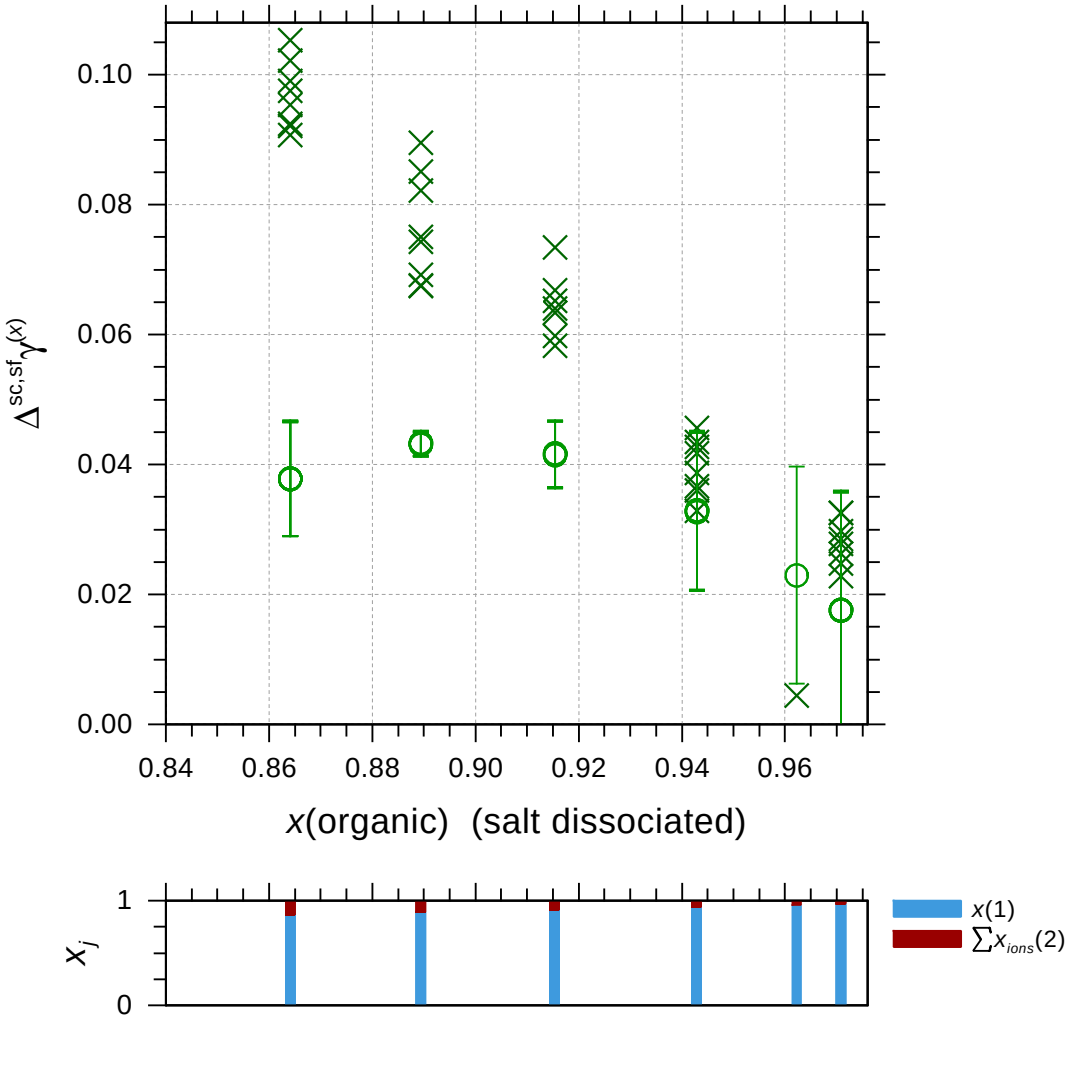


initial weighting of dataset:
$w^{init}(1000)$ = 0.010
dataset contribution to F_{obj}:
fval(1000) = 3.6244E-03
rel. contribution = 0.0017 %

Fig. S0026 (AIOMFAC_output_1001)

1-Butanol (1) + $CaCl_2$ (2)

Temperature range: 374 -- 393 K

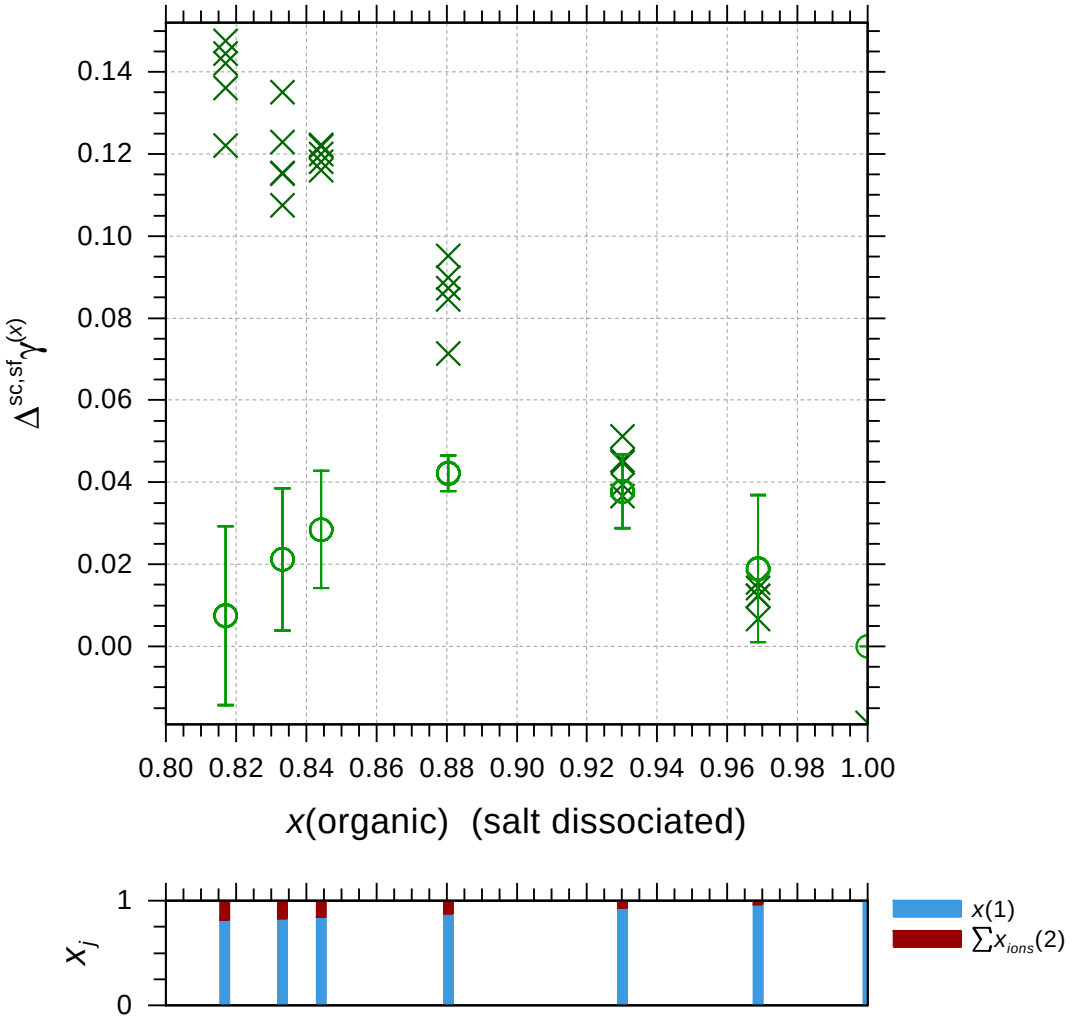


initial weighting of dataset:
$w^{init}(1001)$ = 0.010
dataset contribution to F_{obj}:
fval(1001) = 8.9630E-05
rel. contribution = 0.0000 %

Fig. S0027 (AIOMFAC_output_1007)

Isobutanol (1) + $CaCl_2$ (2)

Temperature range: 373 -- 382 K



initial weighting of dataset:
$w^{init}(1007)$ = 0.010
dataset contribution to F_{obj}:
fval(1007) = 4.6003E-04
rel. contribution = 0.0002 %

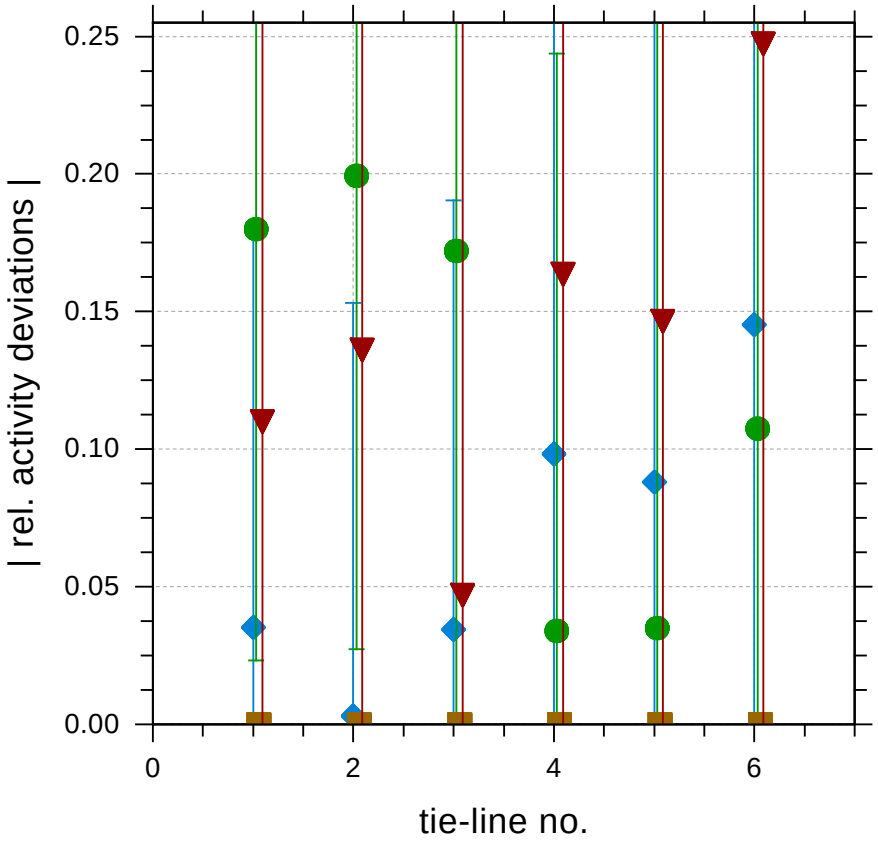
Fig. S0028 (AIOMFAC_output_1009)

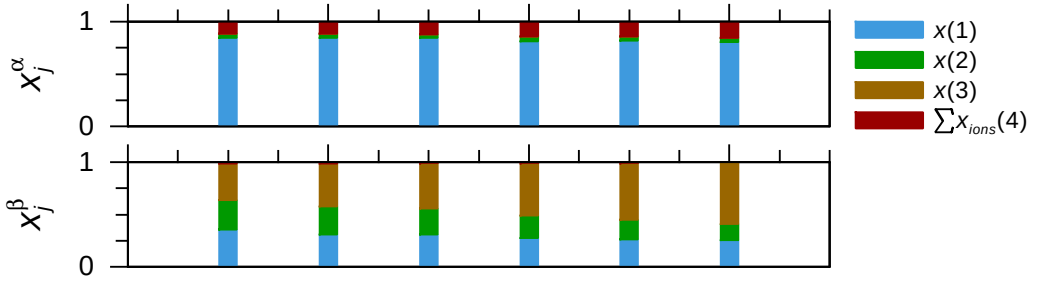
H_2O (1) + Ethanol (2) + 3-Methyl-1-butanol (3) + $CaCl_2$ (4)

Temperature: 298 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



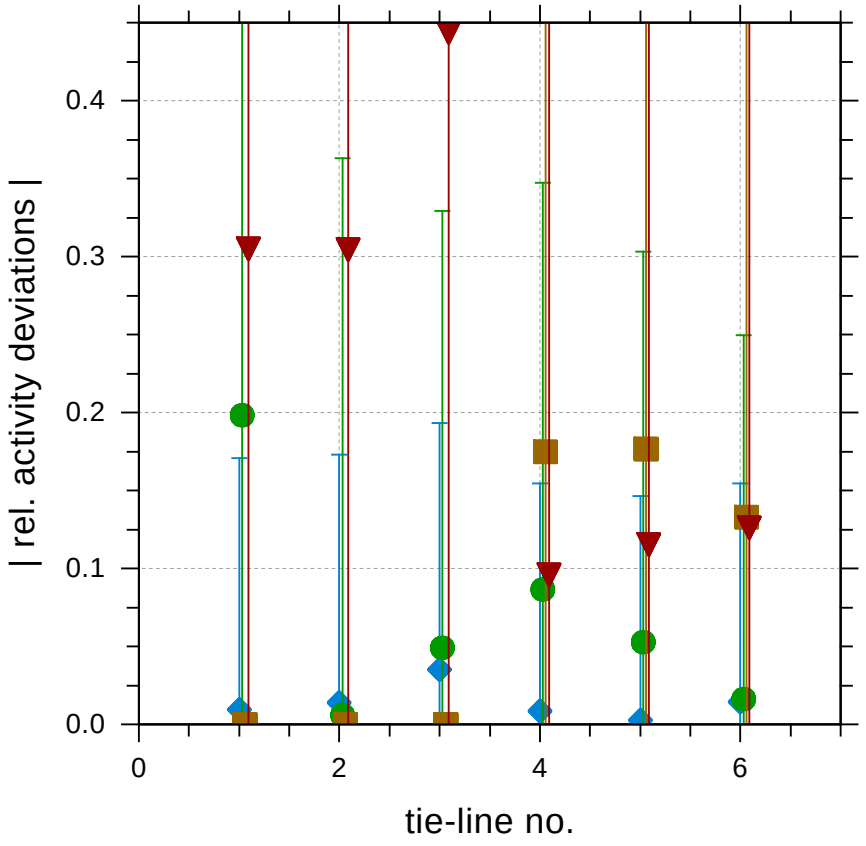


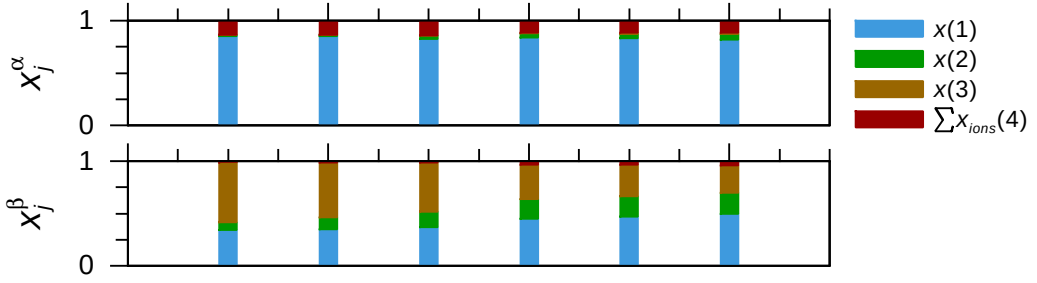
initial weighting of dataset:
w^{init}(1009) = 1.000
dataset contribution to F_{obj}:
fval(1009) = 2.4918E-01
rel. contribution = 0.1185 %

Fig. S0029 (AIOMFAC_output_1010)

H_2O (1) + Ethanol (2) + 1-Butanol (3) + $CaCl_2$ (4)

Temperature: 298 K



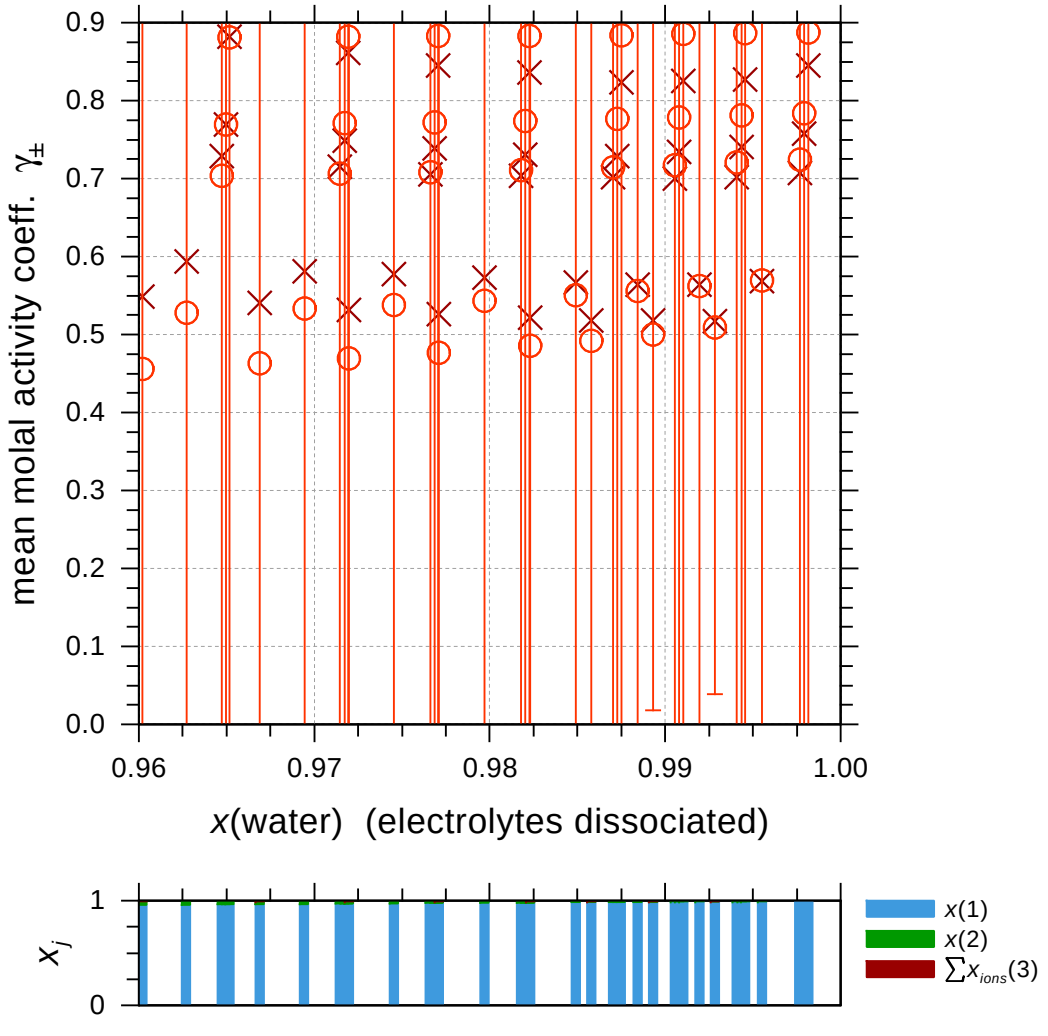


initial weighting of dataset:
w^{init}(1010) = 1.000
dataset contribution to F_{obj}:
fval(1010) = 4.6206E-01
rel. contribution = 0.2197 %

Fig. S0030 (AIOMFAC_output_1040)

H_2O (1) + D-Mannopyranose (2) + $CaCl_2$ (3)

Temperature: 298 K

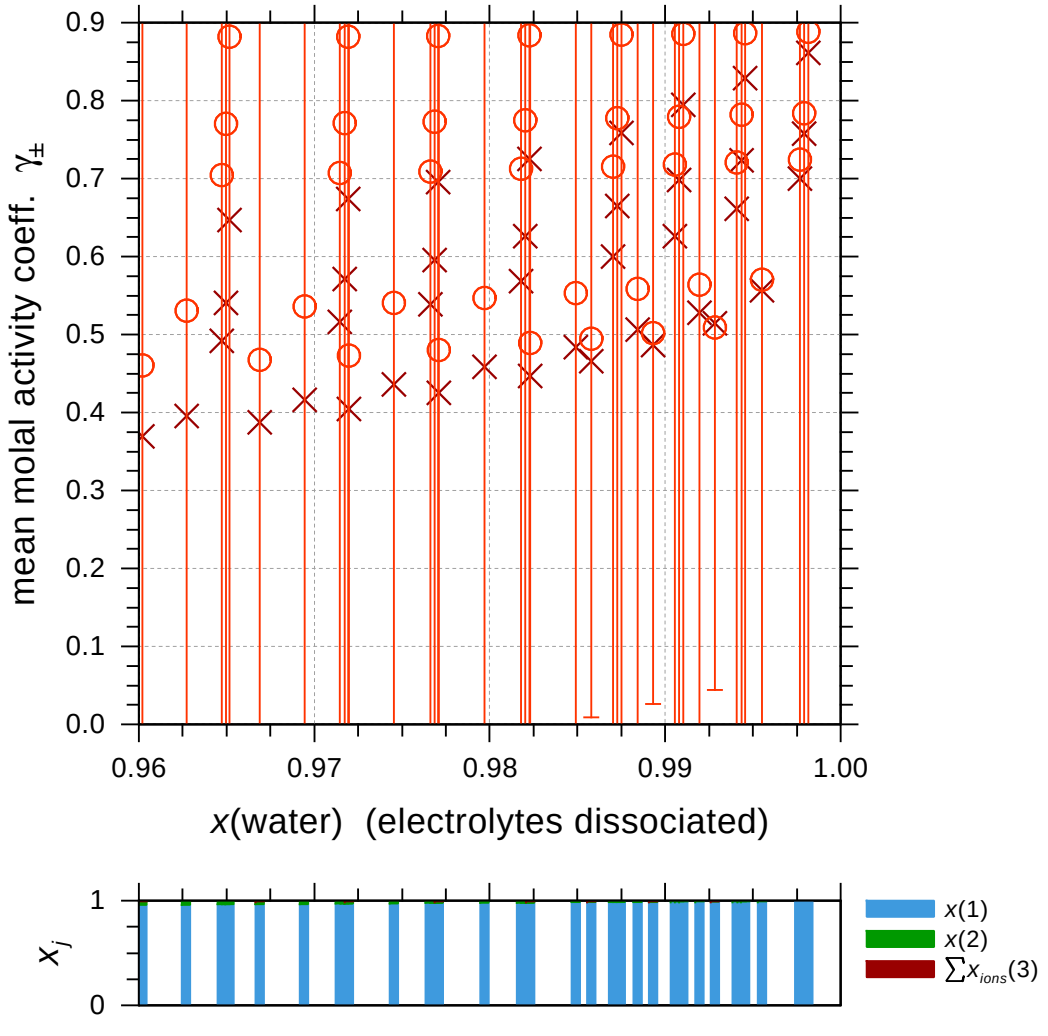


initial weighting of dataset:
$w^{init}(1040)$ = 2.000
dataset contribution to F_{obj}:
fval(1040) = 1.1434E-02
rel. contribution = 0.0054 %

Fig. S0031 (AIOMFAC_output_1043)

H_2O (1) + D-Ribofuranose (2) + $CaCl_2$ (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(1043)$ = 2.000

dataset contribution to F_{obj}:

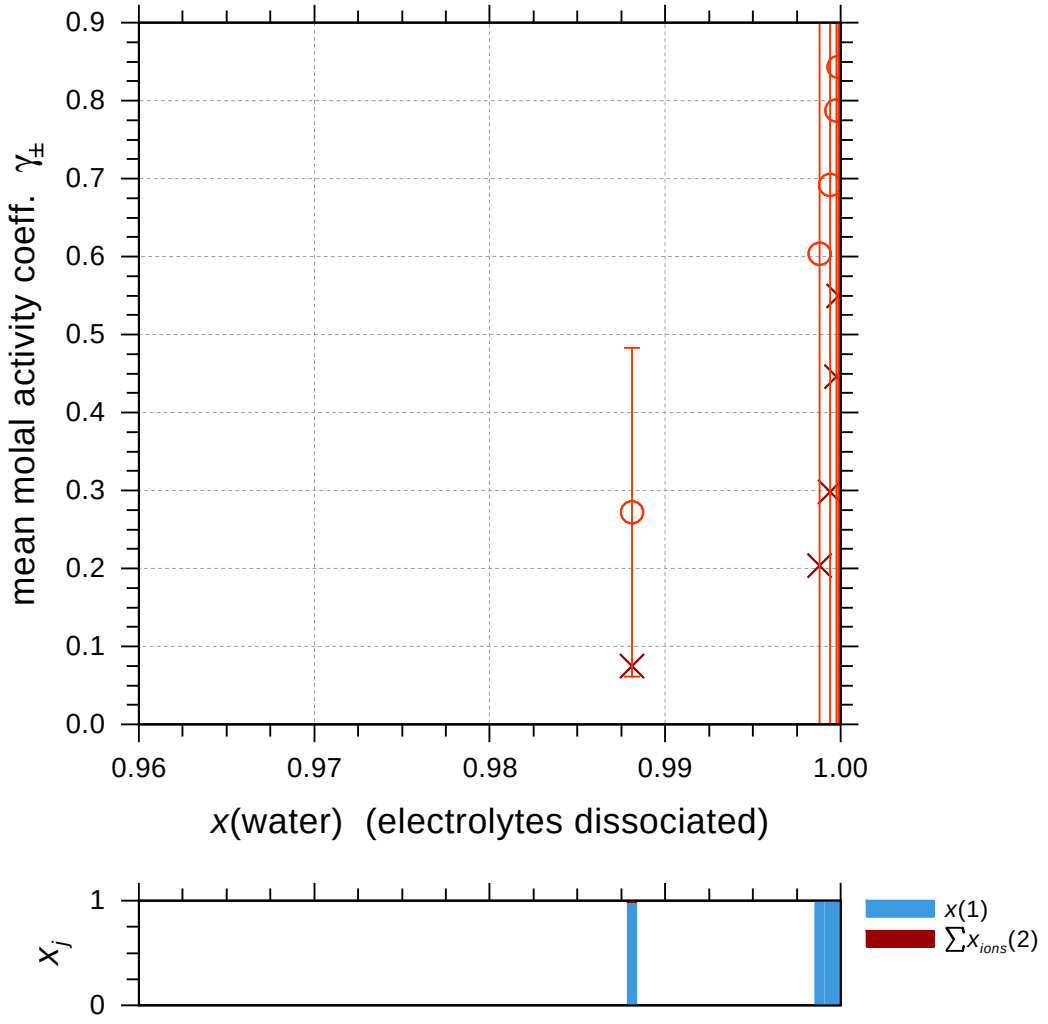
fval(1043) = 2.8993E-02

rel. contribution = 0.0138 %

Fig. S0032 (AIOMFAC_output_1015)

2-Propanol (1) + HCl (2)

Temperature: 298 K

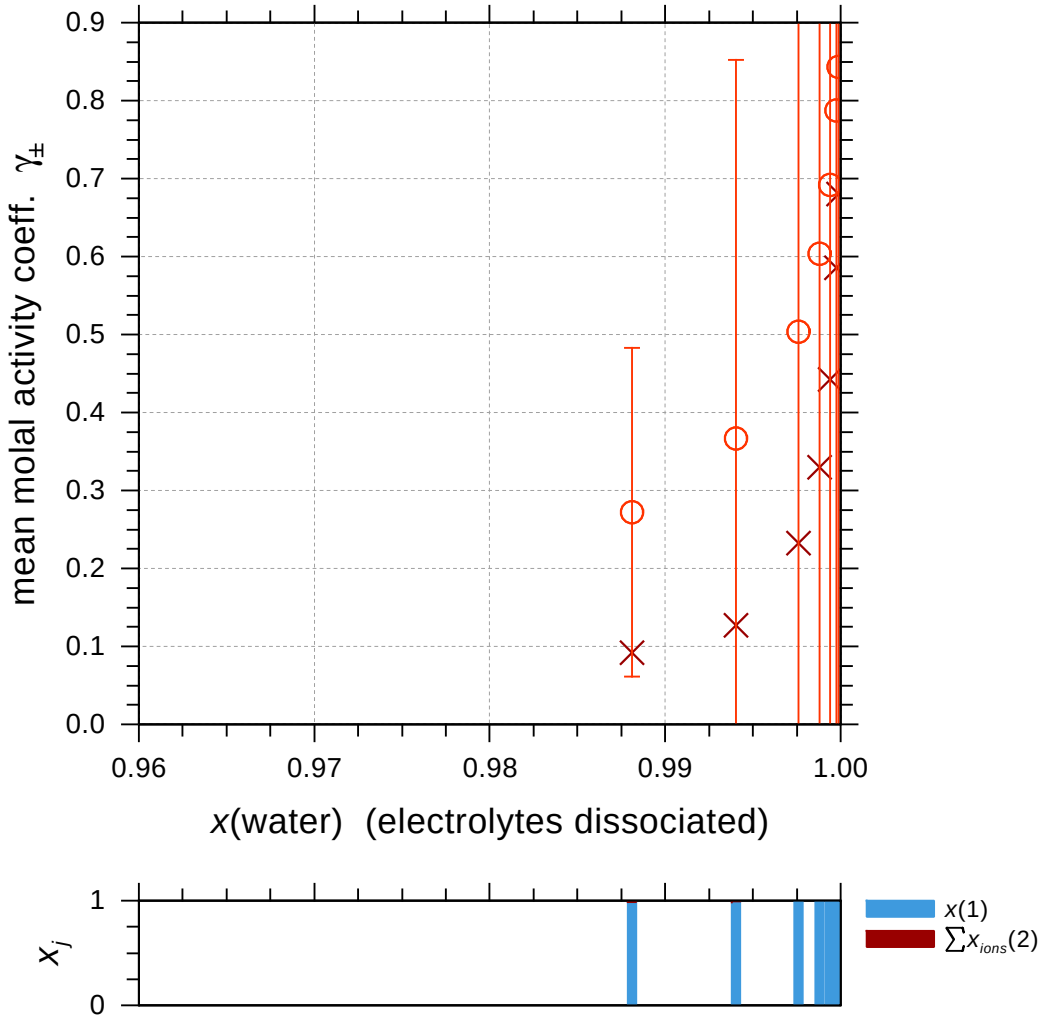


initial weighting of dataset:
$w^{init}(1015)$ = 2.000
dataset contribution to F_{obj}:
fval(1015) = 1.0236E+00
rel. contribution = 0.4867 %

Fig. S0033 (AIOMFAC_output_1016)

1-Propanol (1) + HCl (2)

Temperature: 298 K

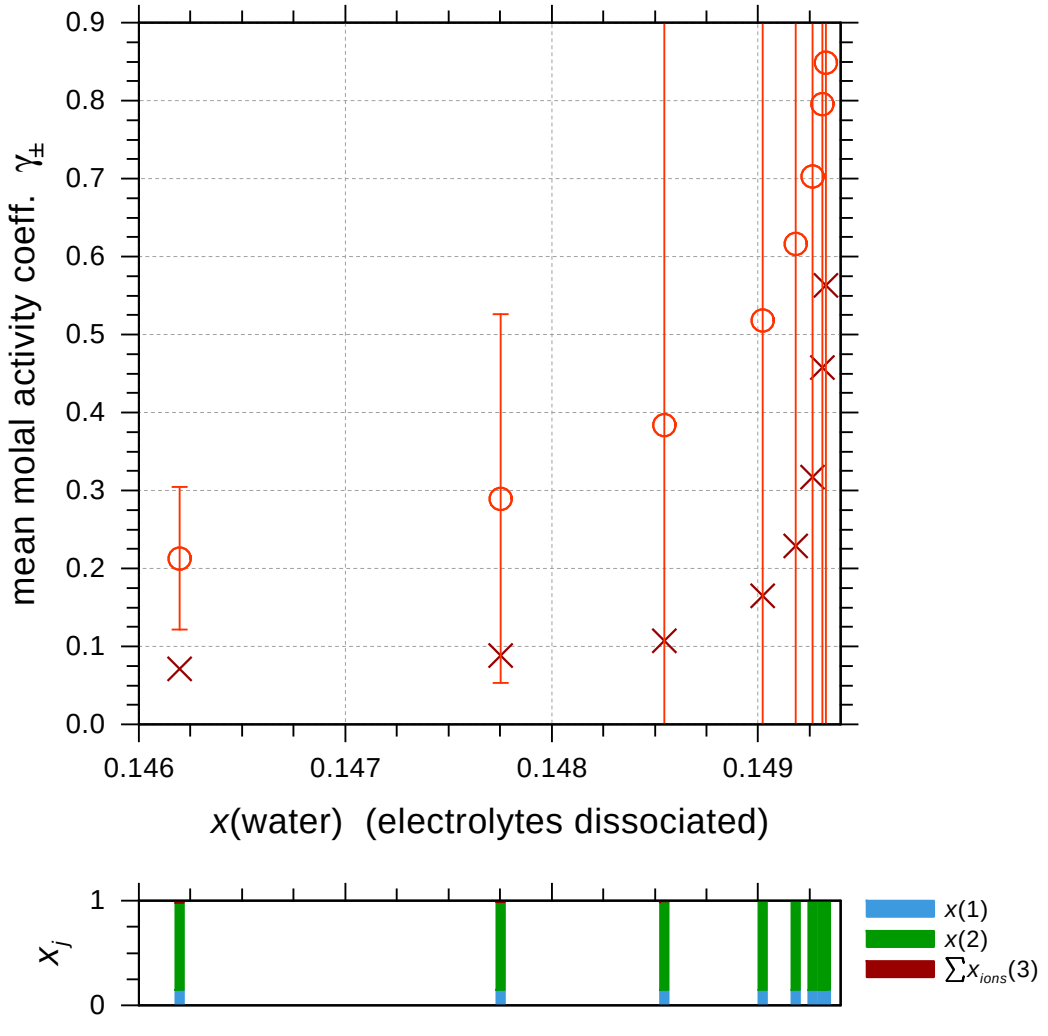


initial weighting of dataset:
$w^{init}(1016)$ = 2.000
dataset contribution to F_{obj}:
fval(1016) = 1.1094E+00
rel. contribution = 0.5275 %

Fig. S0034 (AIOMFAC_output_1017)

H_2O (1) + 2-Propanol (2) + HCl (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(1017)$ = 2.000

dataset contribution to F_{obj}:

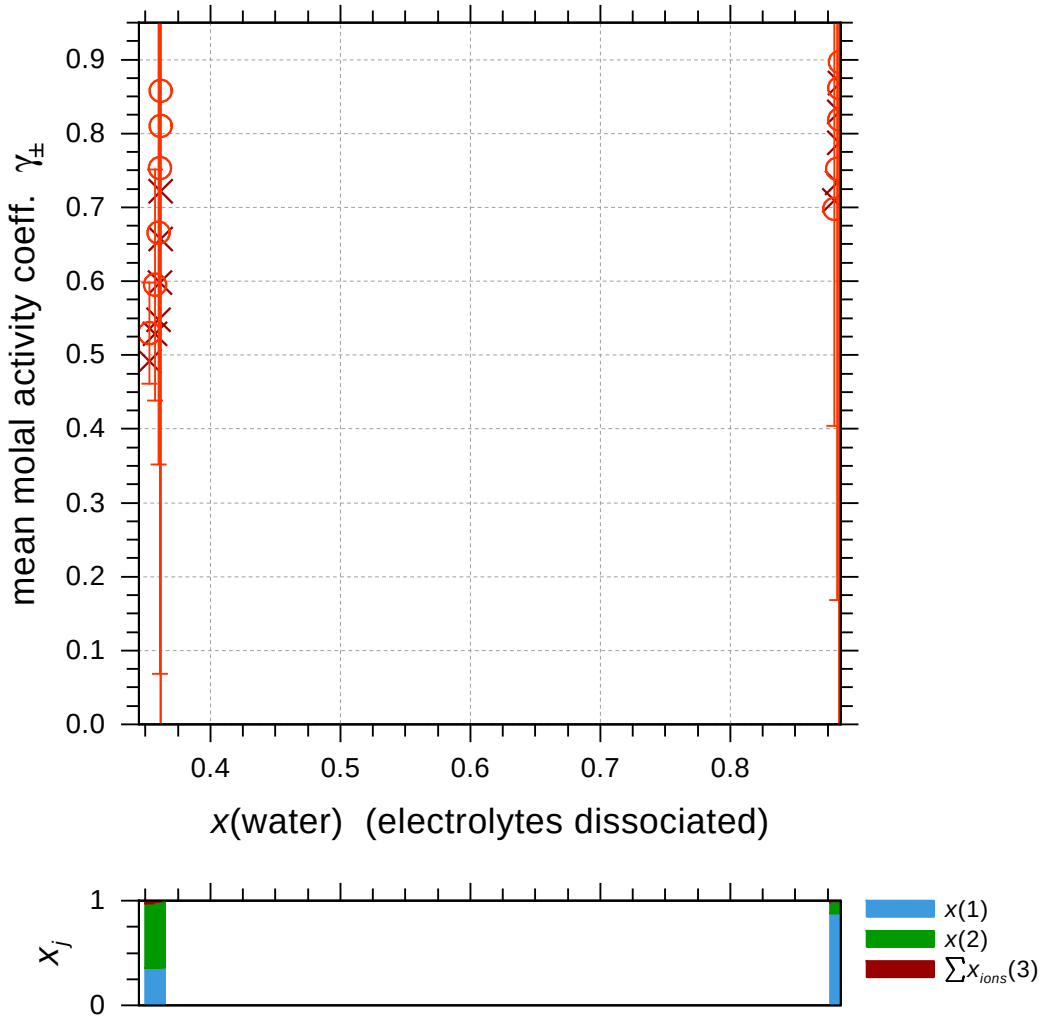
fval(1017) = 2.8363E+00

rel. contribution = 1.3487 %

Fig. S0035 (AIOMFAC_output_1018)

H_2O (1) + Glycerol (2) + HCl (3)

Temperature: 298 K

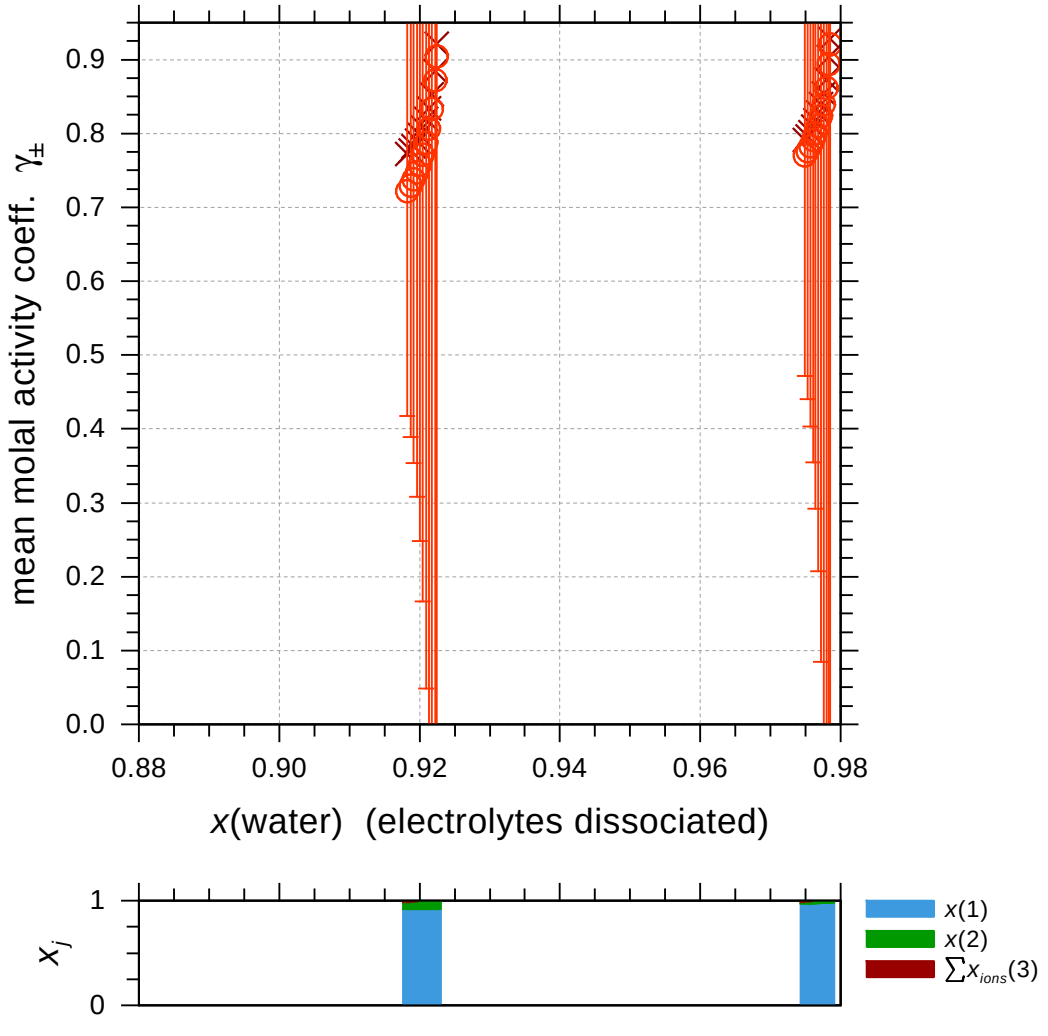


initial weighting of dataset:
$w^{init}(1018)$ = 2.000
dataset contribution to F_{obj}:
fval(1018) = 1.0504E-01
rel. contribution = 0.0500 %

Fig. S0036 (AIOMFAC_output_1019)

H_2O (1) + Glycerol (2) + HCl (3)

Temperature: 298 K

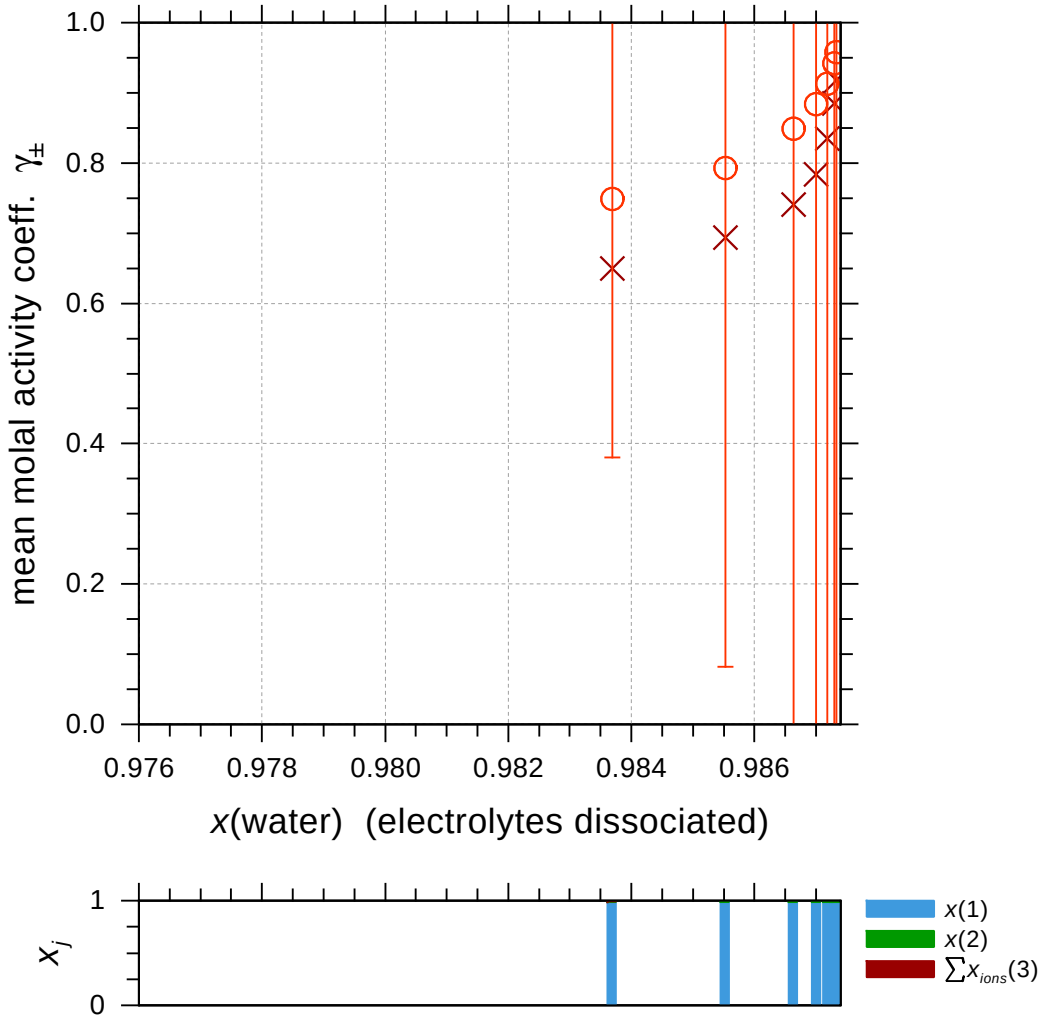


initial weighting of dataset:
$w^{init}(1019)$ = 2.000
dataset contribution to F_{obj}:
fval(1019) = 9.8628E-03
rel. contribution = 0.0047 %

Fig. S0037 (AIOMFAC_output_1020)

H_2O (1) + 1-Butanol (2) + HCl (3)

Temperature: 298 K

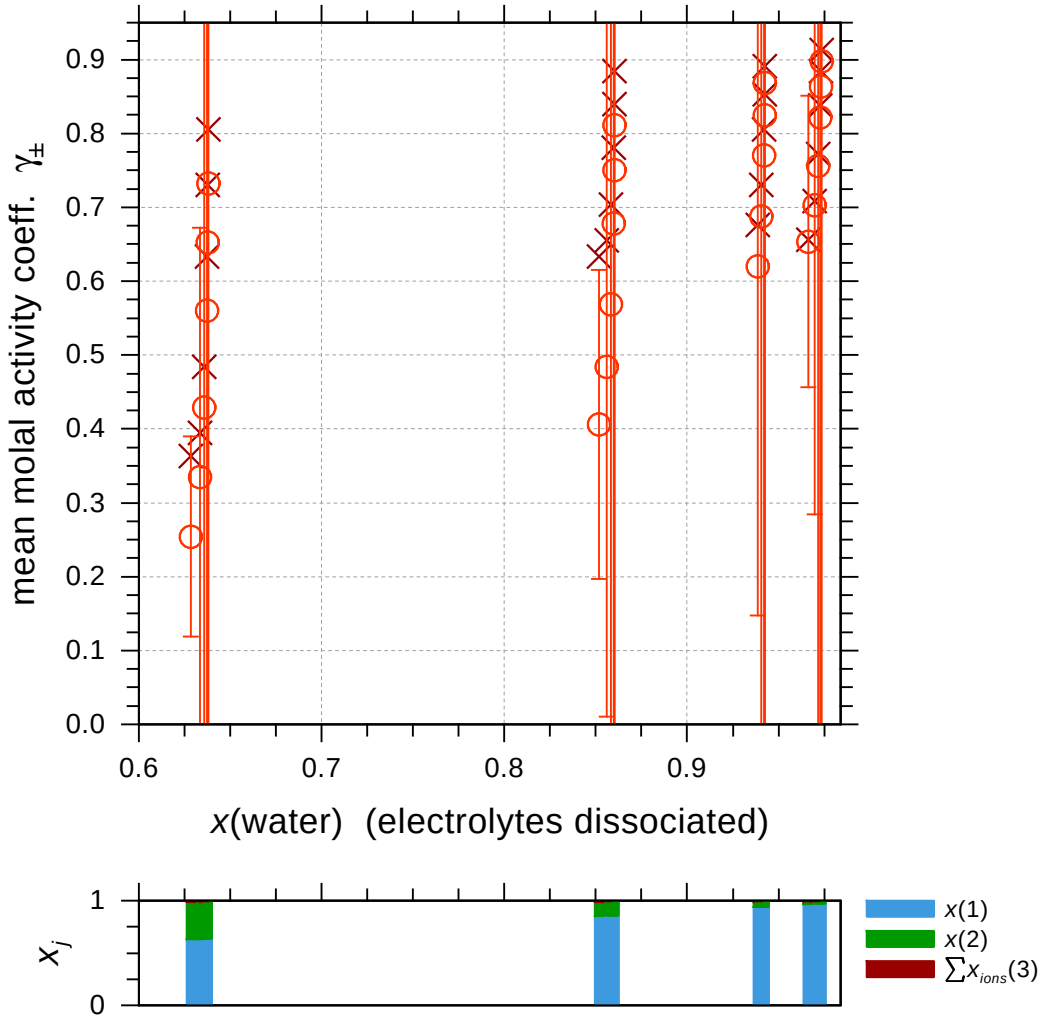


initial weighting of dataset:
$w^{init}(1020)$ = 2.000
dataset contribution to F_{obj}:
fval(1020) = 3.5719E-02
rel. contribution = 0.0170 %

Fig. S0038 (AIOMFAC_output_1021)

H_2O (1) + *tert*-Butanol (2) + HCl (3)

Temperature: 298 K

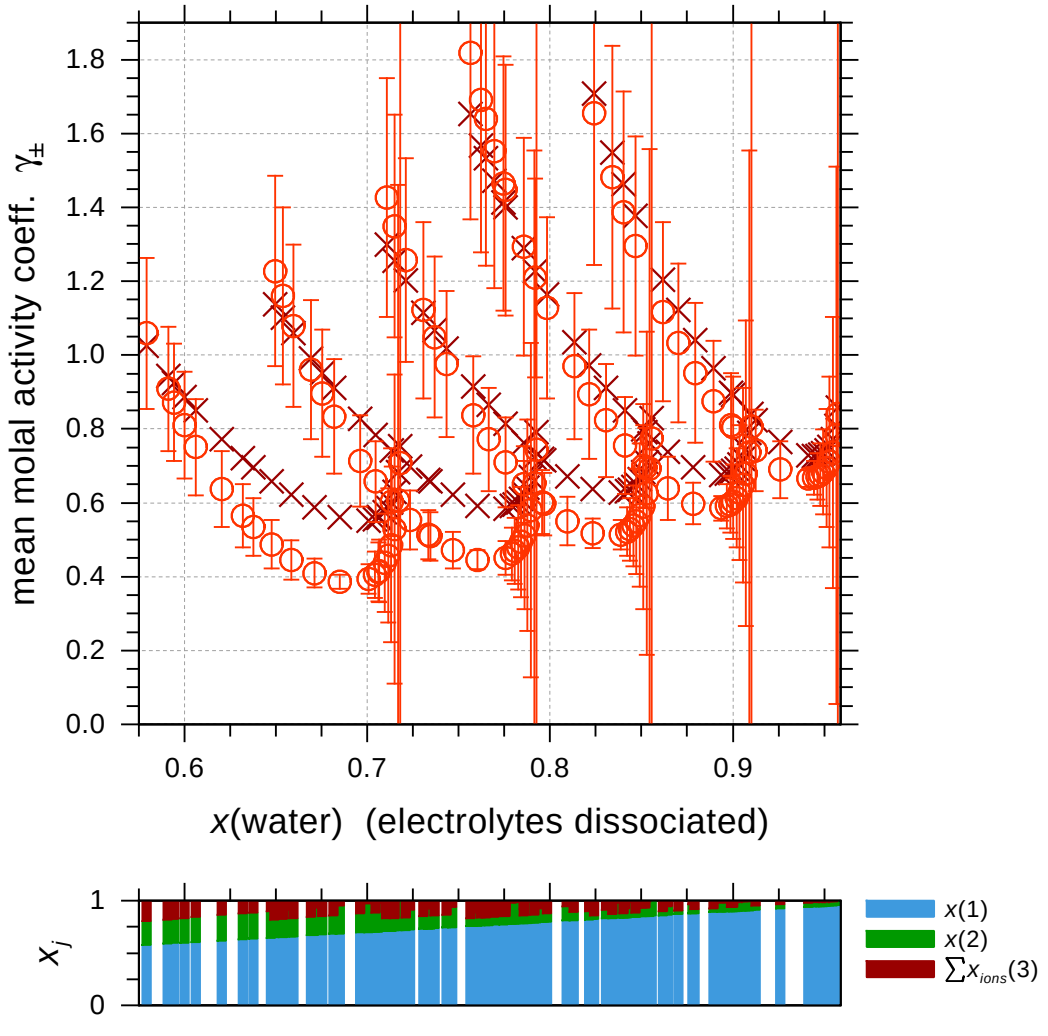


initial weighting of dataset:
$w^{init}(1021)$ = 2.000
dataset contribution to F_{obj}:
fval(1021) = 1.4349E-01
rel. contribution = 0.0682 %

Fig. S0039 (AIOMFAC_output_1048)

H_2O (1) + Ethanol (2) + HCl (3)

Temperature: 298 K

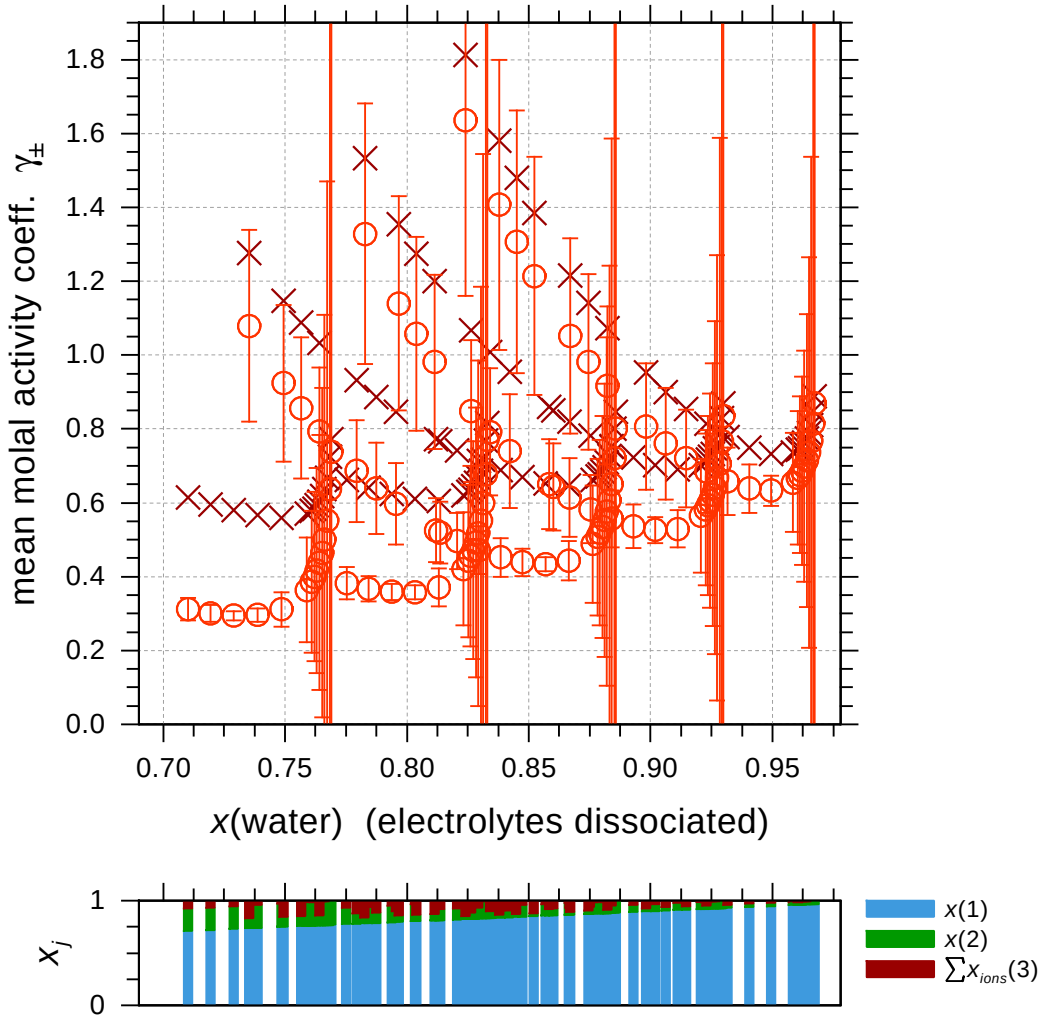


initial weighting of dataset:
$w^{init}(1048)$ = 2.000
dataset contribution to F_{obj}:
fval(1048) = 3.0613E-01
rel. contribution = 0.1456 %

Fig. S0040 (AIOMFAC_output_1049)

H_2O (1) + 2-Propanol (2) + HCl (3)

Temperature: 298 K

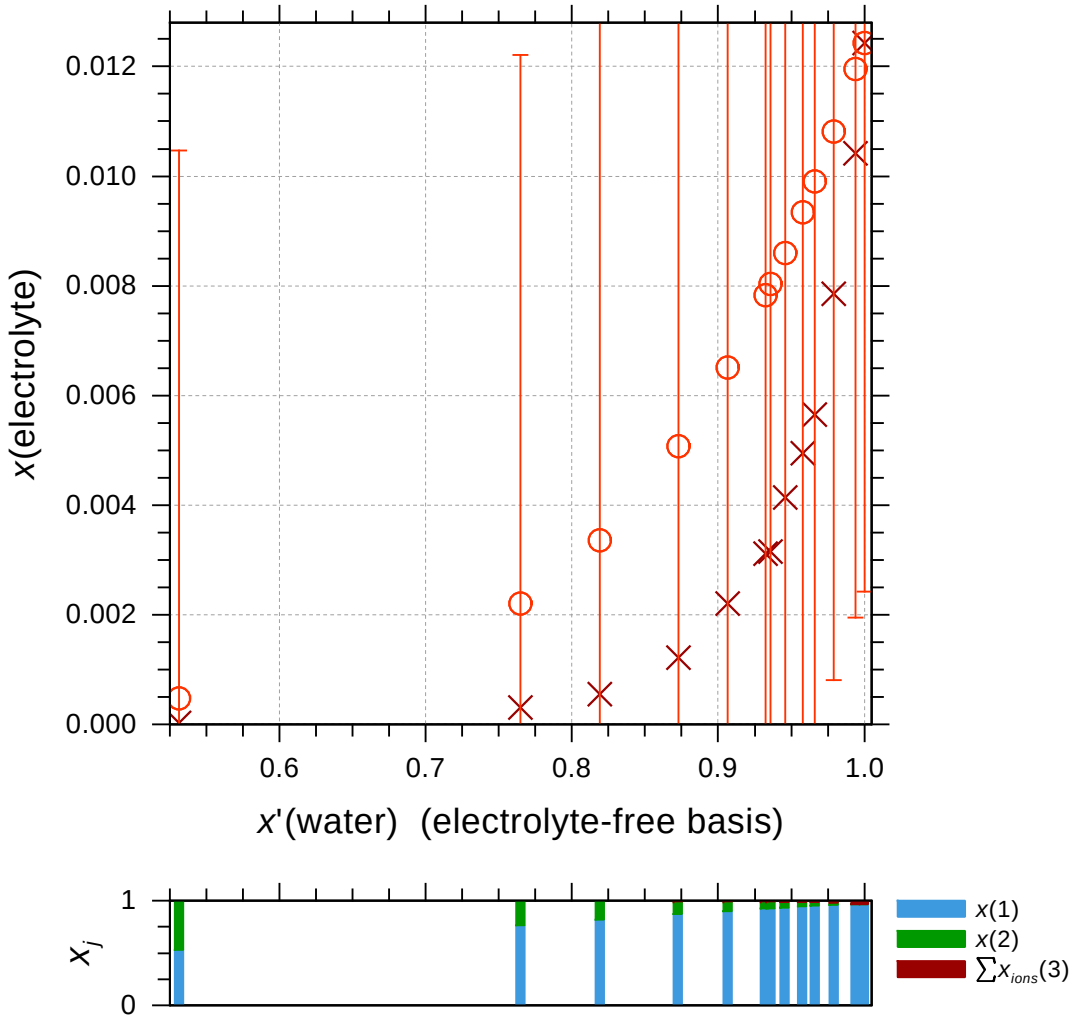


initial weighting of dataset:
$w^{init}(1049)$ = 2.000
dataset contribution to F_{obj}:
fval(1049) = 8.7367E-01
rel. contribution = 0.4155 %

Fig. S0041 (AIOMFAC_output_0079)

H_2O (1) + Ethanol (2) + K_2SO_4 (3)

Temperature: 298 K

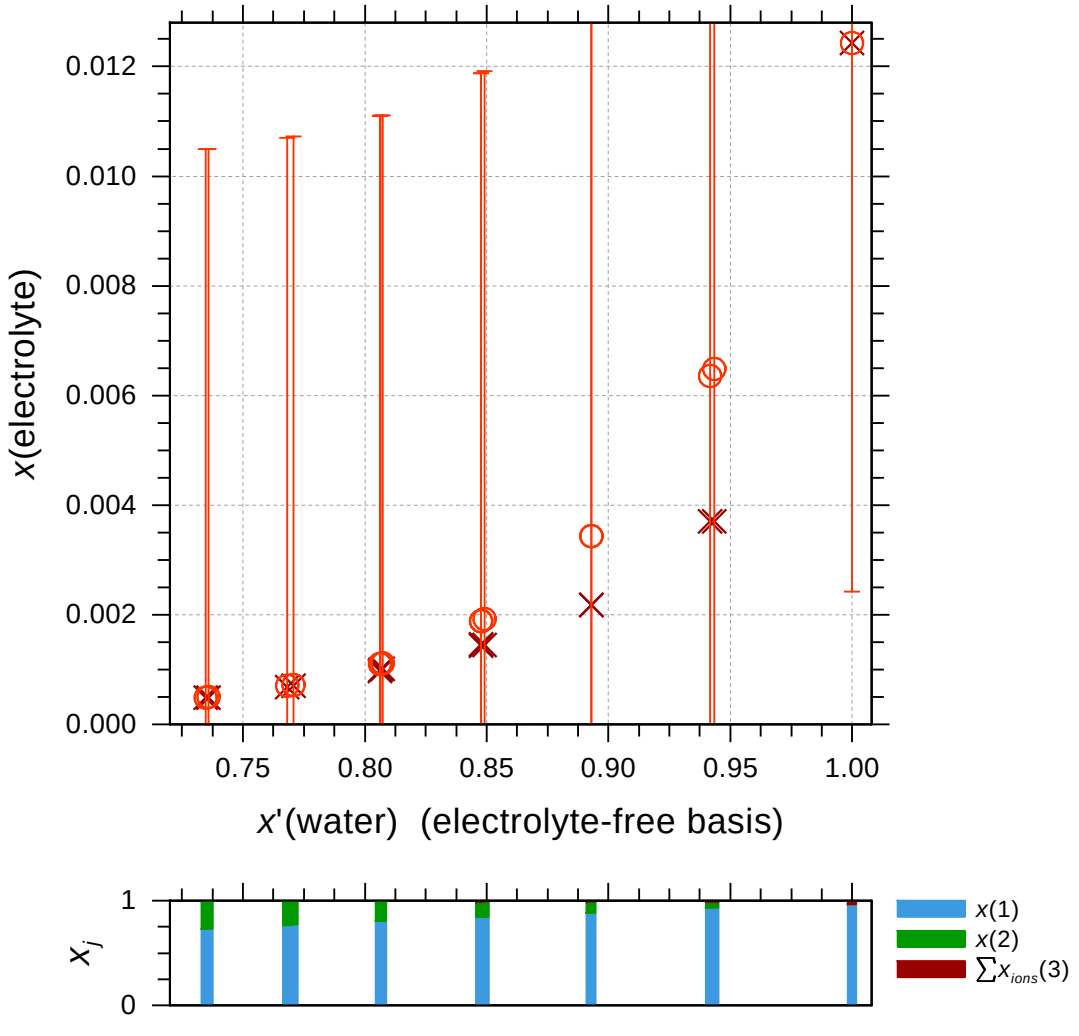


initial weighting of dataset:
$w^{init}(0079)$ = 1.000
dataset contribution to F_{obj}:
fval(0079) = 6.9962E-01
rel. contribution = 0.3327 %

Fig. S0042 (AIOMFAC_output_0080)

H_2O (1) + 1-Propanol (2) + K_2SO_4 (3)

Temperature: 298 K

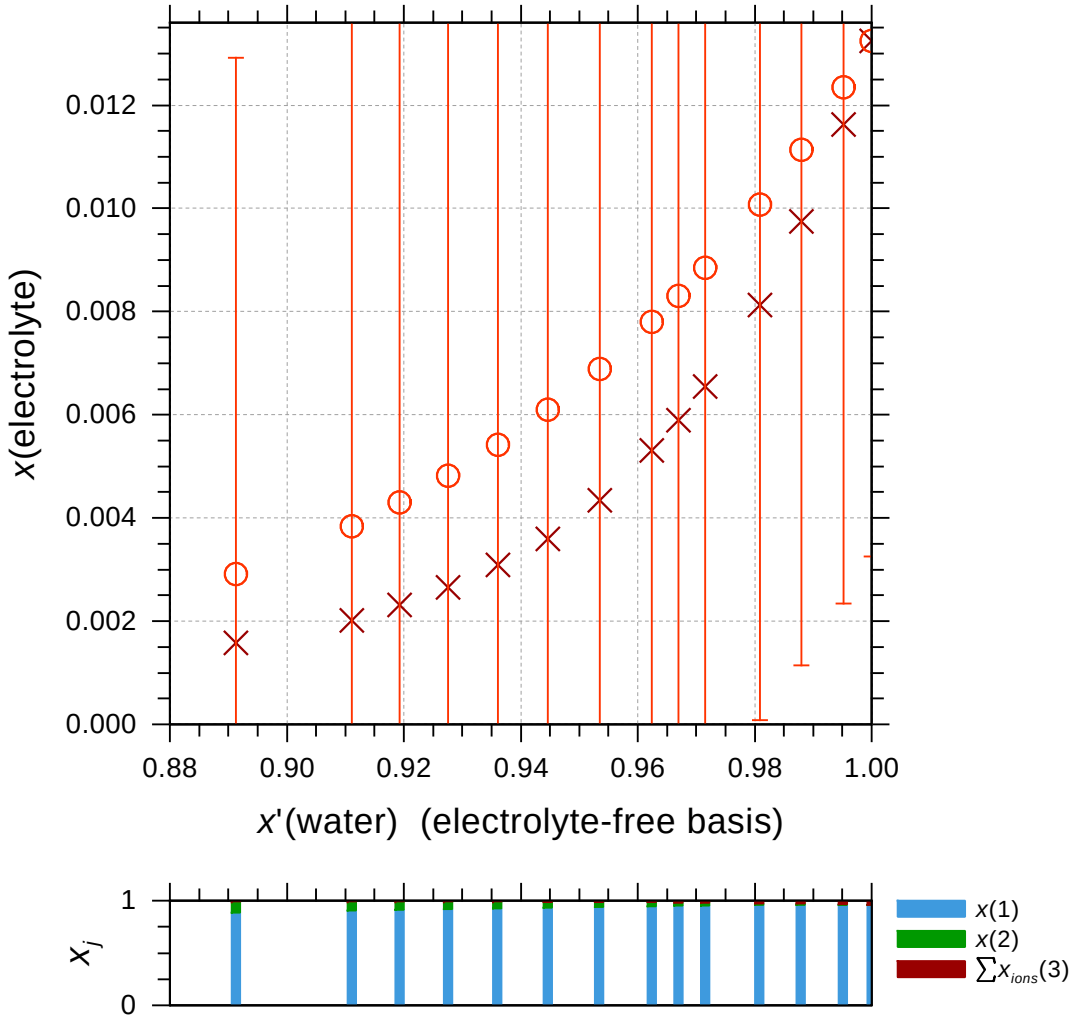


initial weighting of dataset:
$w^{init}(0080)$ = 1.000
dataset contribution to F_{obj}:
fval(0080) = 7.0319E-02
rel. contribution = 0.0334 %

Fig. S0043 (AIOMFAC_output_0081)

H_2O (1) + 2-Propanol (2) + K_2SO_4 (3)

Temperature: 303 K

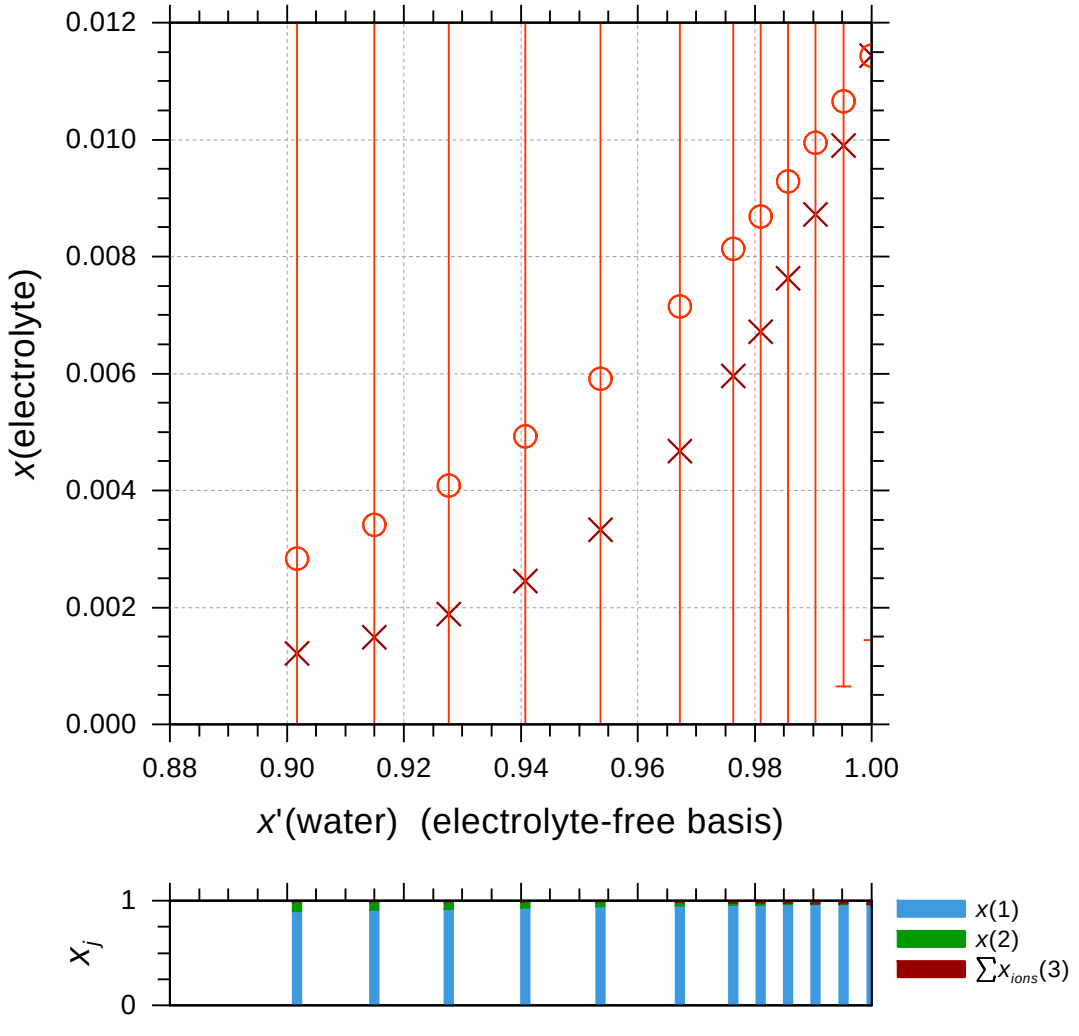


initial weighting of dataset:
$w^{init}(0081)$ = 1.000
dataset contribution to F_{obj}:
fval(0081) = 1.9632E-01
rel. contribution = 0.0934 %

Fig. S0044 (AIOMFAC_output_0971)

H_2O (1) + 2-Propanol (2) + K_2SO_4 (3)

Temperature: 293 K

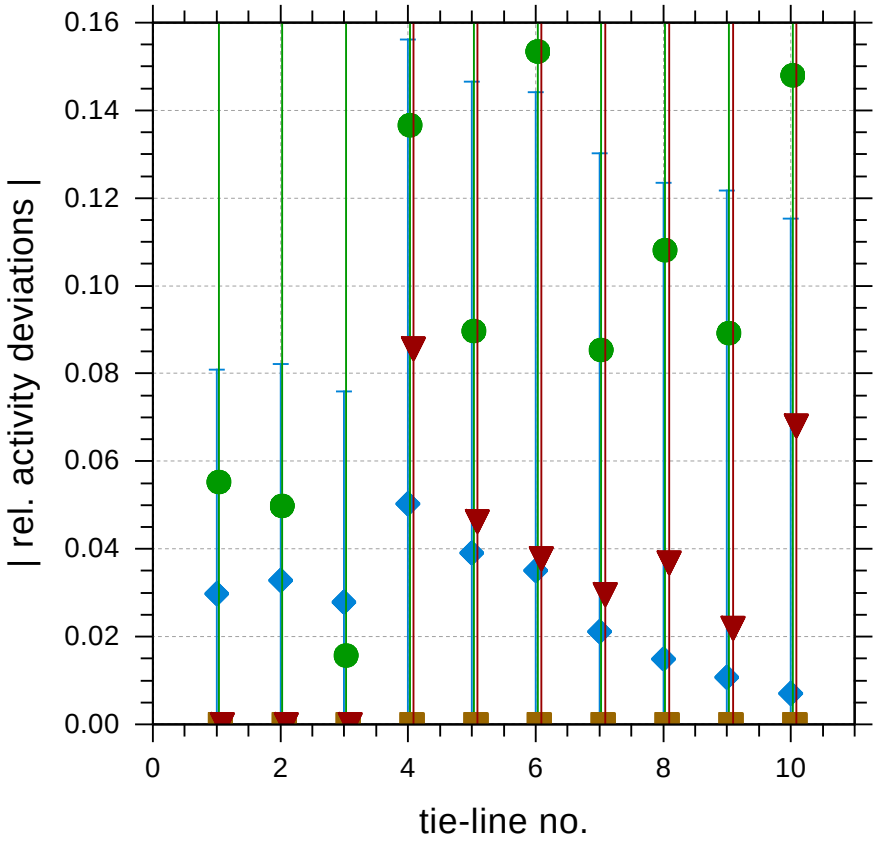


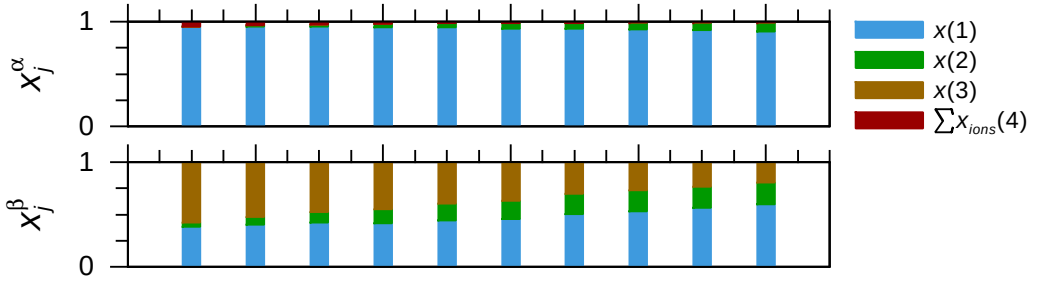
initial weighting of dataset:
w^{init}(0971) = 0.800
dataset contribution to F_{obj}:
fval(0971) = 1.5667E-01
rel. contribution = 0.0745 %

Fig. S0045 (AIOMFAC_output_1014)

H_2O (1) + Ethanol (2) + 1-Pentanol (3) + K_2SO_4 (4)

Temperature: 298 K



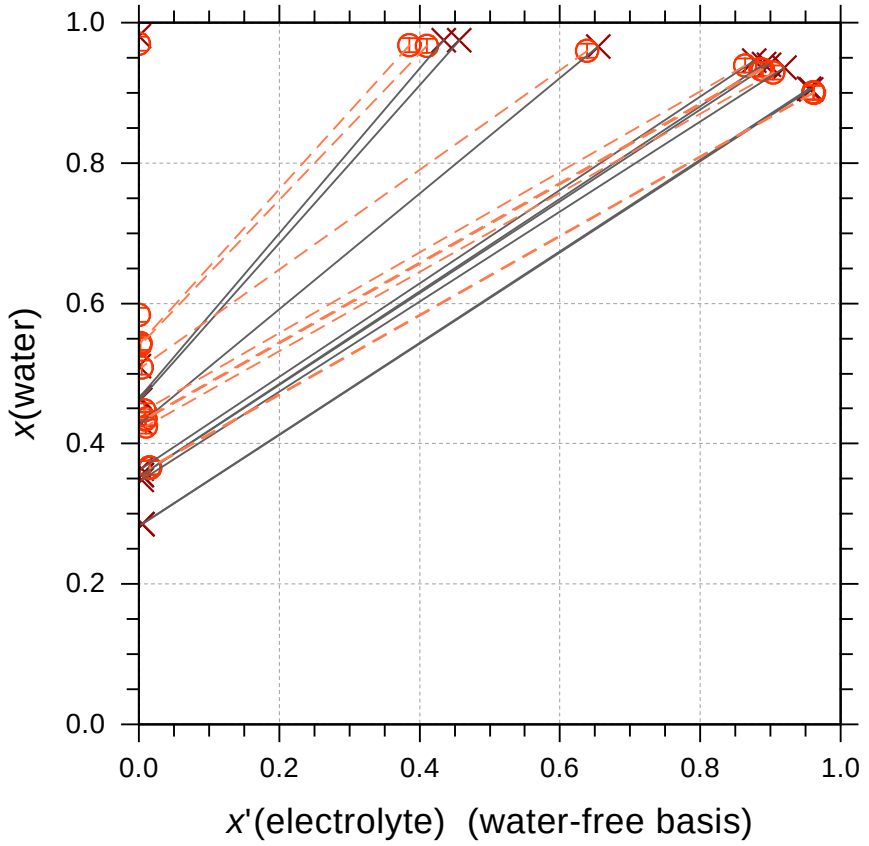


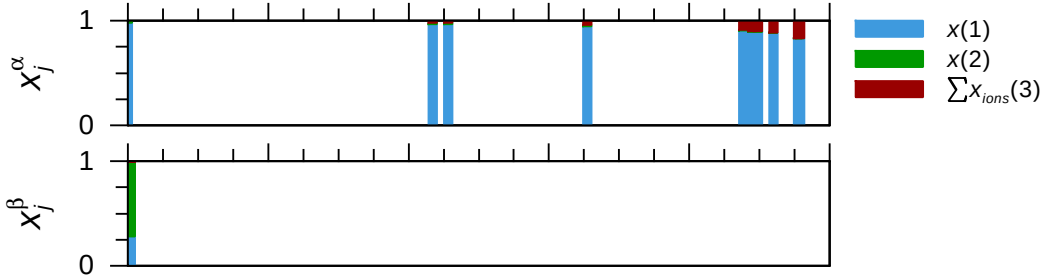
initial weighting of dataset:
$w^{init}(1014)$ = 1.000
dataset contribution to F_{obj}:
fval(1014) = 6.5963E-02
rel. contribution = 0.0314 %

Fig. S0046 (AIOMFAC_output_0105)

H_2O (1) + 1-Butanol (2) + KBr (3)

Temperature: 323 K





left y-axis:

× KBr_1-BuOH_LLE_Li

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0105)$ = 1.000

dataset contribution to F_{obj}:

fval(0105) = 1.8738E-01

rel. contribution = 0.0891 %

Fig. S0046a (AIOMFAC_output_0105)

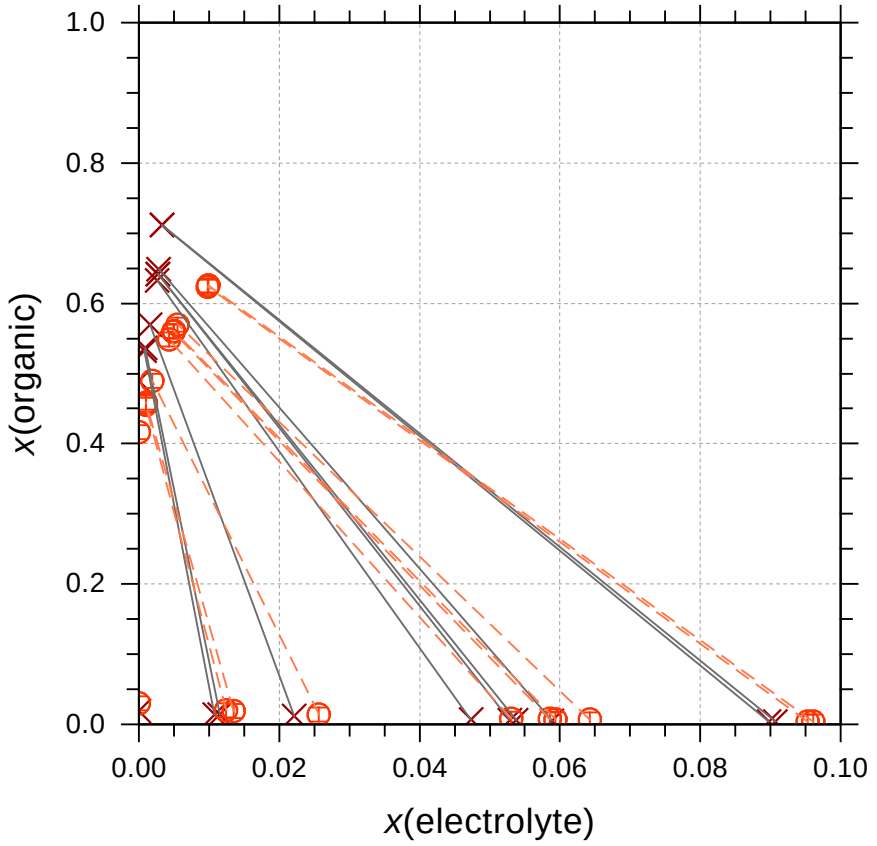
H_2O (1) + 1-Butanol (2) + KBr (3)

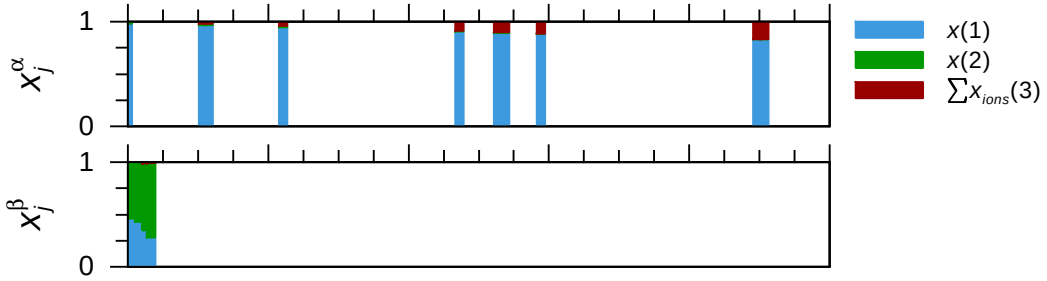
Temperature: 323 K

left y-axis:

× KBr_1-BuOH_LLE_Li

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0105)$ = 1.000

dataset contribution to F_{obj}:

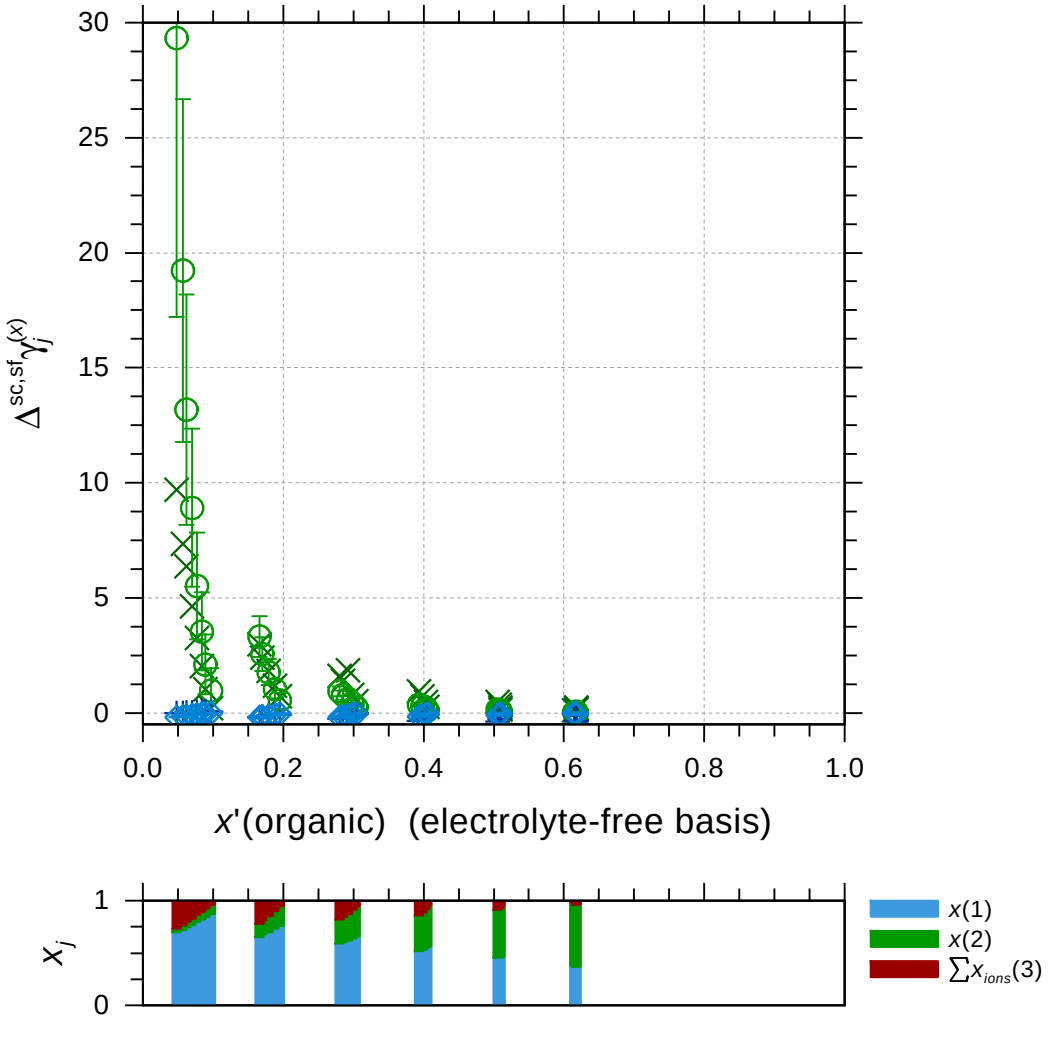
fval(0105) = 1.8738E-01

rel. contribution = 0.0891 %

Fig. S0047 (AIOMFAC_output_0106)

H_2O (1) + 1-Propanol (2) + KBr (3)

Temperature range: 360 -- 363 K

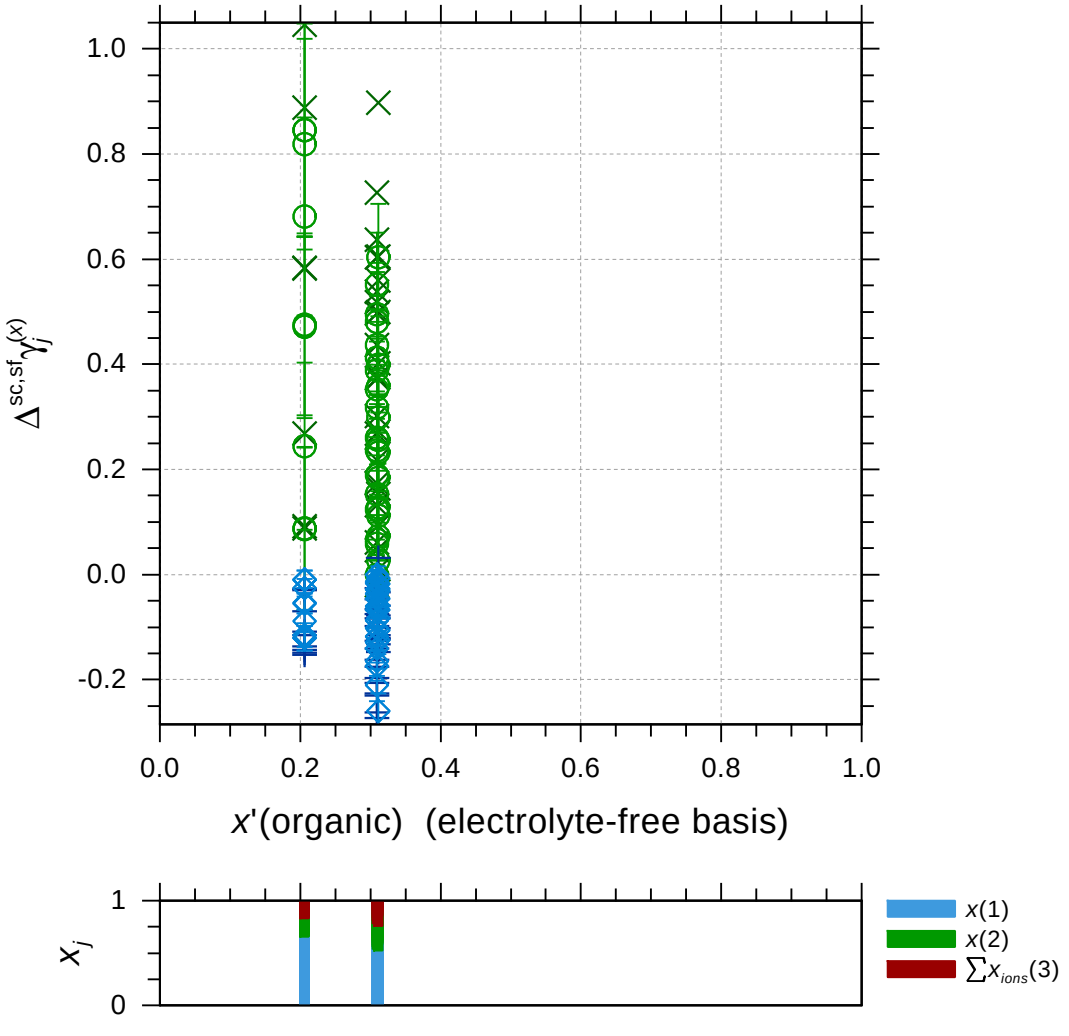


initial weighting of dataset:
$w^{init}(0106)$ = 0.050
dataset contribution to F_{obj}:
fval(0106) = 5.6690E-02
rel. contribution = 0.0270 %

Fig. S0048 (AIOMFAC_output_0107)

H_2O (1) + Ethanol (2) + KBr (3)

Temperature range: 355 -- 357 K

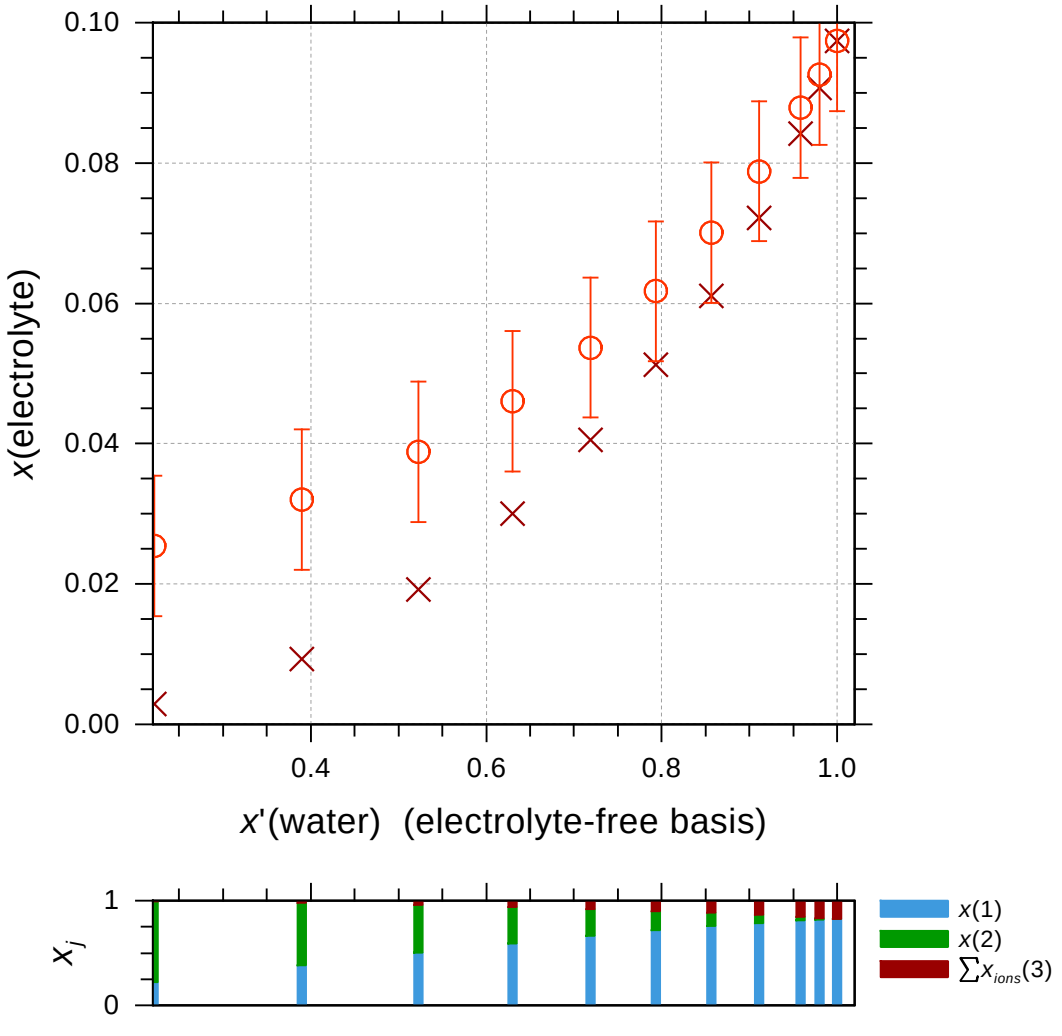


initial weighting of dataset:
$w^{init}(0107)$ = 0.500
dataset contribution to F_{obj}:
fval(0107) = 4.6504E-02
rel. contribution = 0.0221 %

Fig. S0049 (AIOMFAC_output_0108)

H_2O (1) + Ethanol (2) + KBr (3)

Temperature: 303 K



initial weighting of dataset:
$w^{init}(0108)$ = 0.100
dataset contribution to F_{obj}:
fval(0108) = 4.6900E-01
rel. contribution = 0.2230 %

Fig. S0050 (AIOMFAC_output_0974)

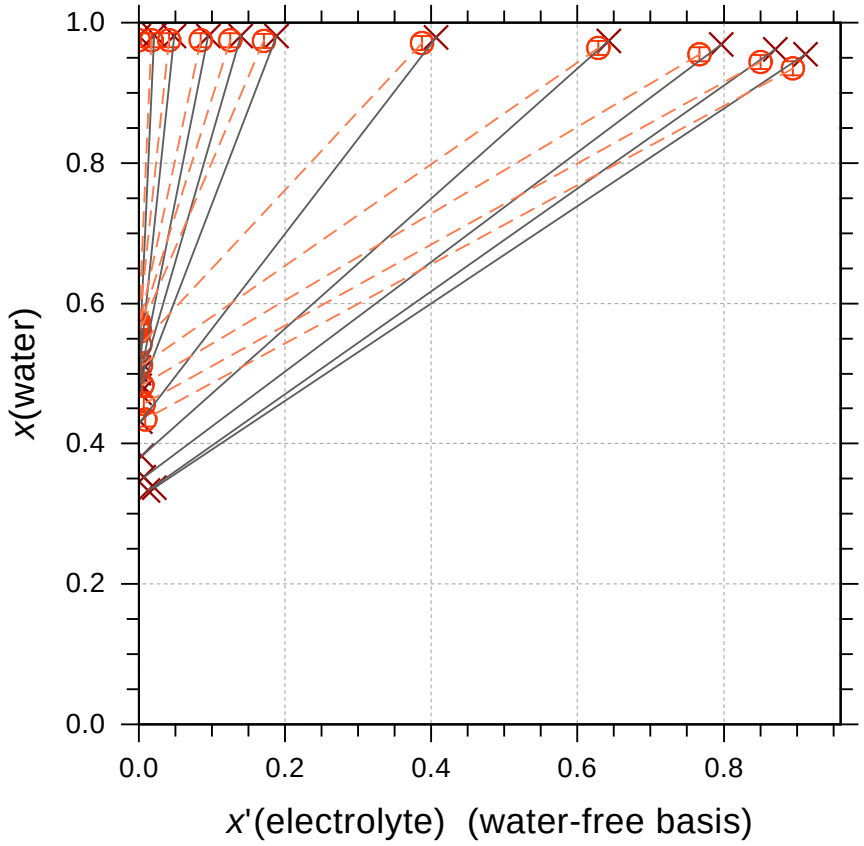
H_2O (1) + 1-Butanol (2) + KBr (3)

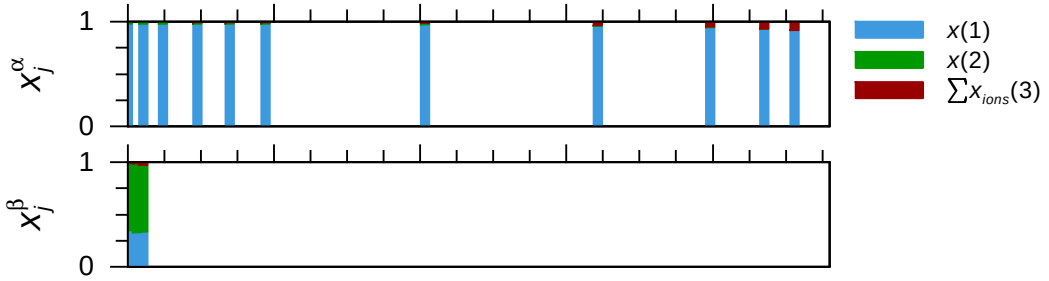
Temperature: 298 K

left y-axis:

× KBr+1-Butanol+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0974)$ = 1.000

dataset contribution to F_{obj}:

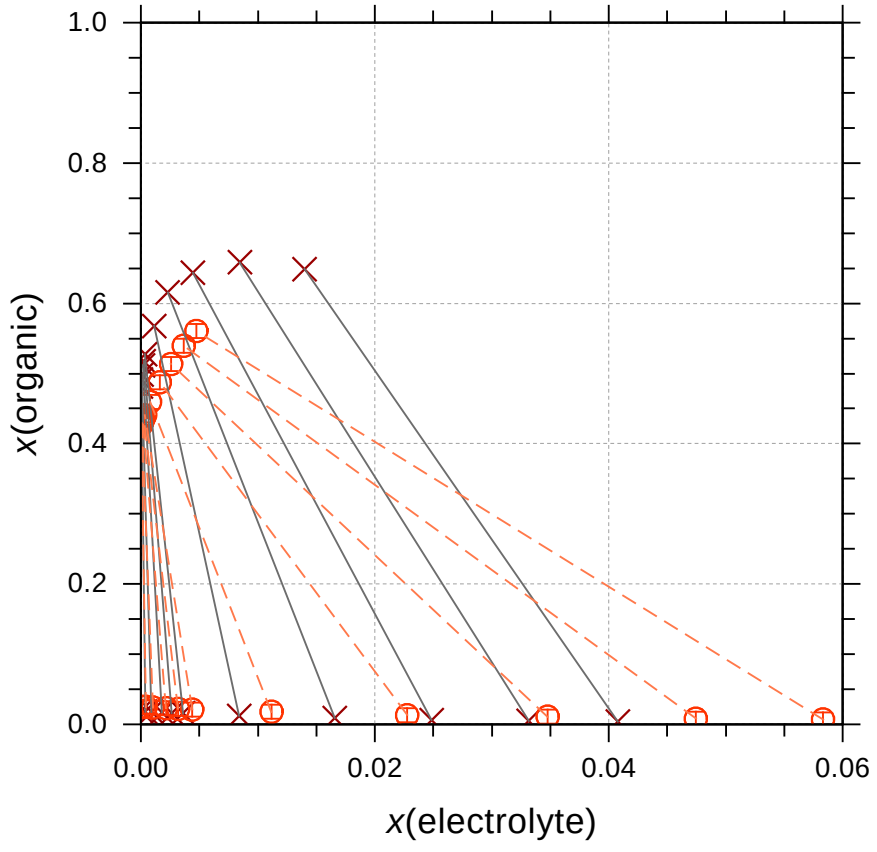
fval(0974) = 7.4530E-01

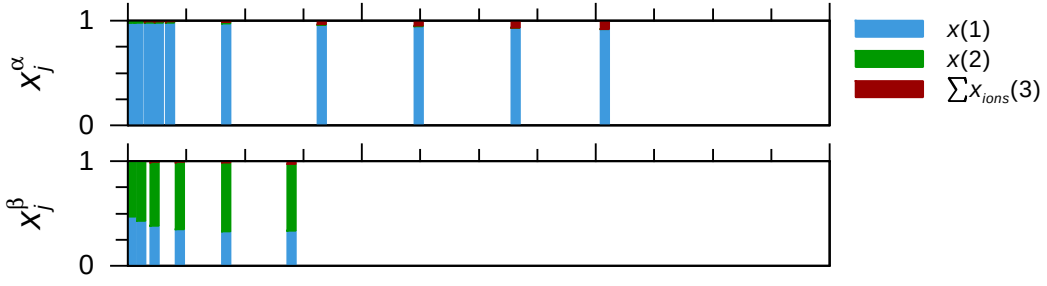
rel. contribution = 0.3544 %

Fig. S0050a (AIOMFAC_output_0974)

H_2O (1) + 1-Butanol (2) + KBr (3)

Temperature: 298 K





left y-axis:

× KBr+1-Butanol+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0974) = 1.000

dataset contribution to F_{obj}:

fval(0974) = 7.4530E-01

rel. contribution = 0.3544 %

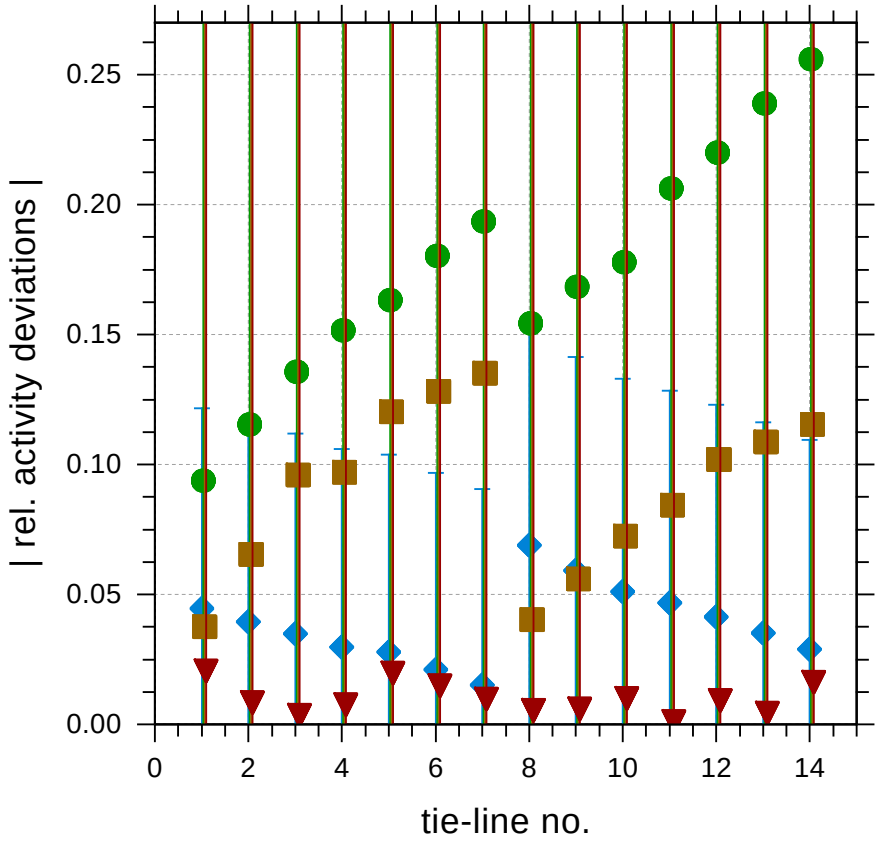
Fig. S0051 (AIOMFAC_output_0976)

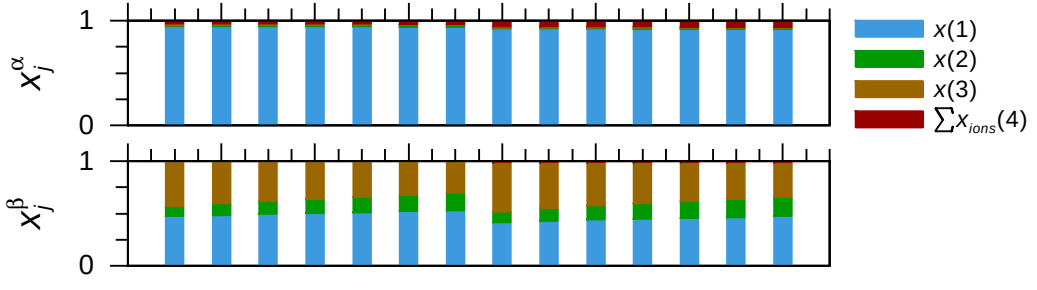
H_2O (1) + *tert*-Butanol (2) + 1-Butanol (3) + KBr (4)

Temperature: 293 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)





initial weighting of dataset:
w^{init}(0976) = 1.000
dataset contribution to F_{obj}:
fval(0976) = 2.1761E-01
rel. contribution = 0.1035 %

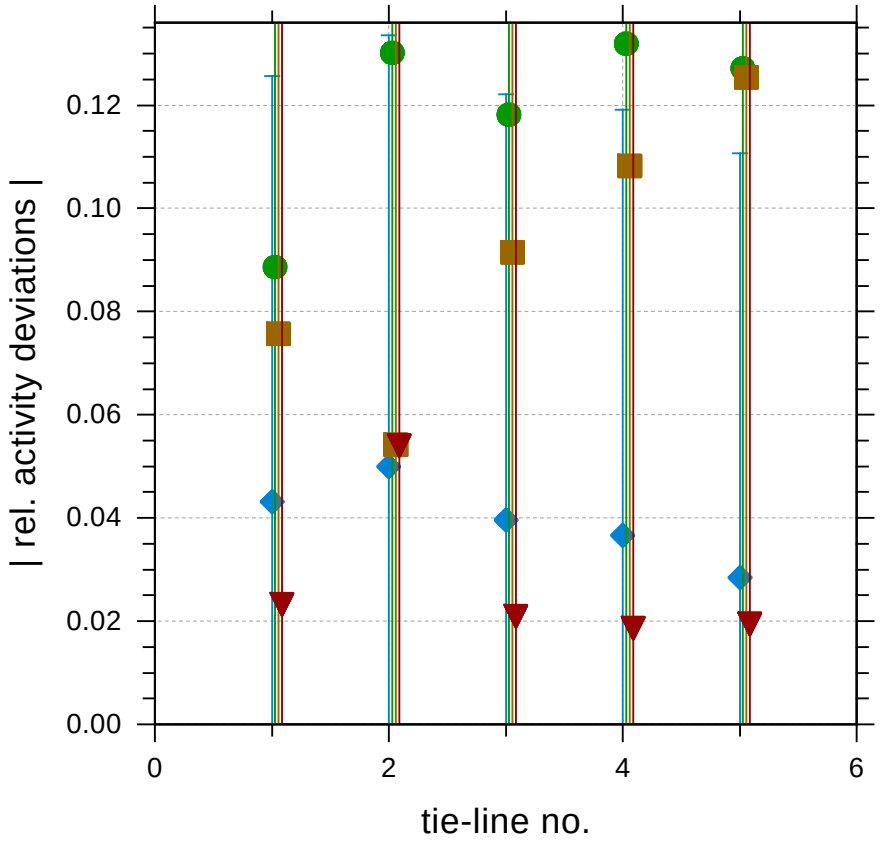
Fig. S0052 (AIOMFAC_output_0977)

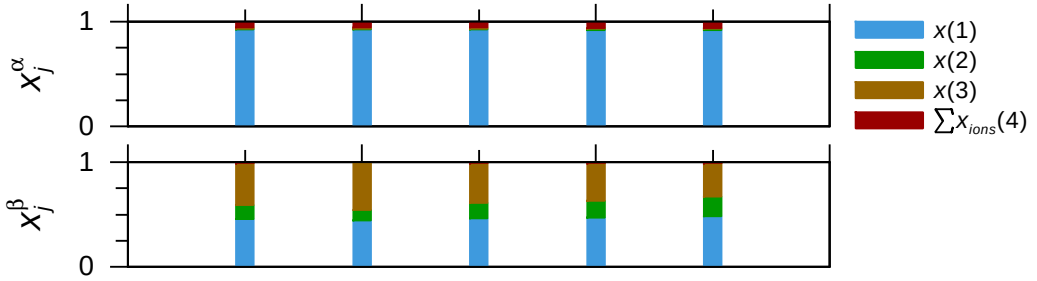
H_2O (1) + *tert*-Butanol (2) + 1-Butanol (3) + KBr (4)

Temperature: 313 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



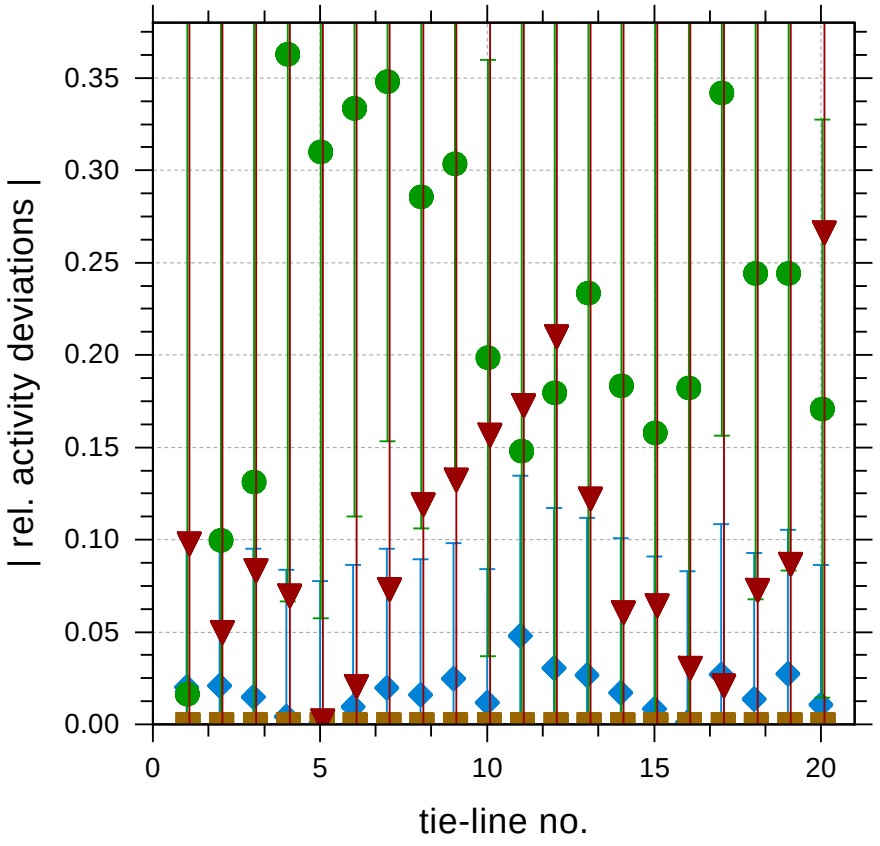


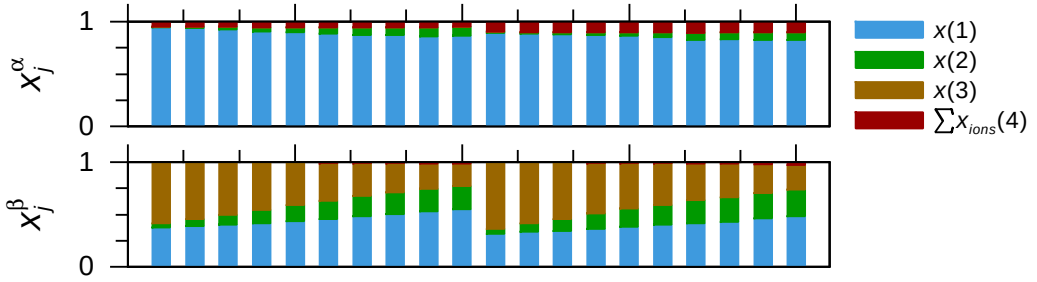
initial weighting of dataset:
$w^{init}(0977)$ = 1.000
dataset contribution to F_{obj}:
fval(0977) = 1.2946E-01
rel. contribution = 0.0616 %

Fig. S0053 (AIOMFAC_output_1013)

H_2O (1) + Ethanol (2) + 1-Pentanol (3) + KBr (4)

Temperature: 298 K



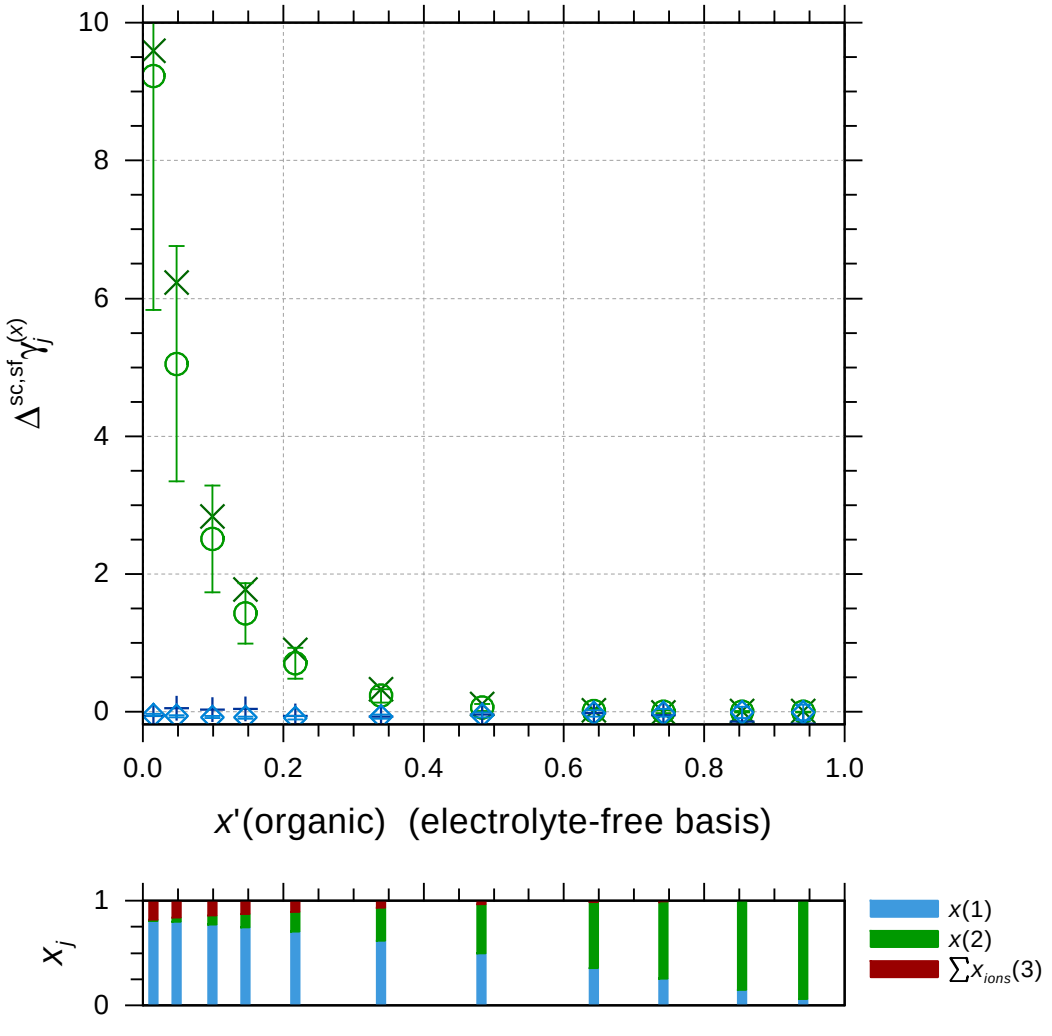


initial weighting of dataset:
$w^{init}(1013)$ = 1.000
dataset contribution to F_{obj}:
fval(1013) = 3.6063E-01
rel. contribution = 0.1715 %

Fig. S0054 (AIOMFAC_output_0028)

H_2O (1) + Ethanol (2) + KCl (3)

Temperature range: 351 -- 369 K

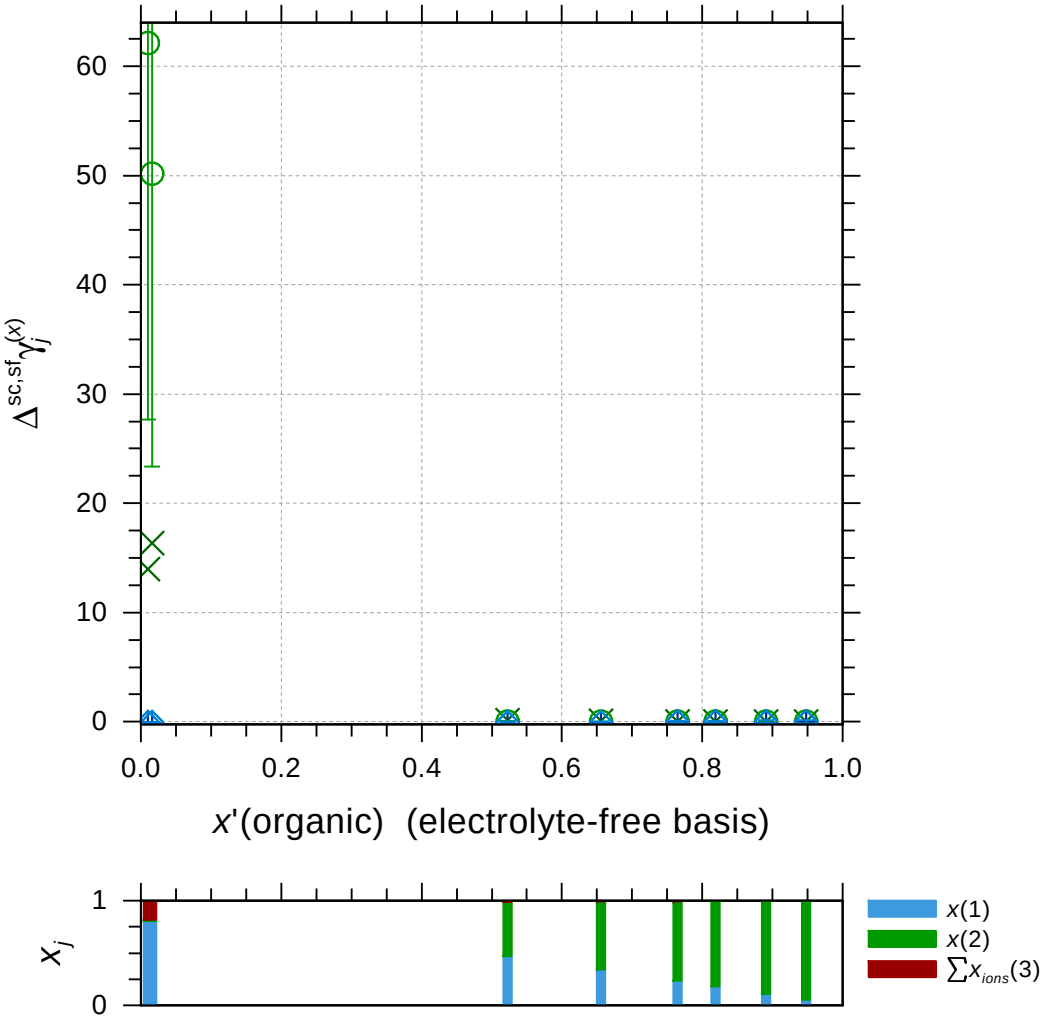


initial weighting of dataset:
$w^{init}(0028)$ = 0.500
dataset contribution to F_{obj}:
fval(0028) = 5.3166E-02
rel. contribution = 0.0253 %

Fig. S0055 (AIOMFAC_output_0029)

H_2O (1) + 1-Propanol (2) + KCl (3)

Temperature range: 362 -- 372 K



initial weighting of dataset:

$w^{init}(0029)$ = 0.500

dataset contribution to F_{obj}:

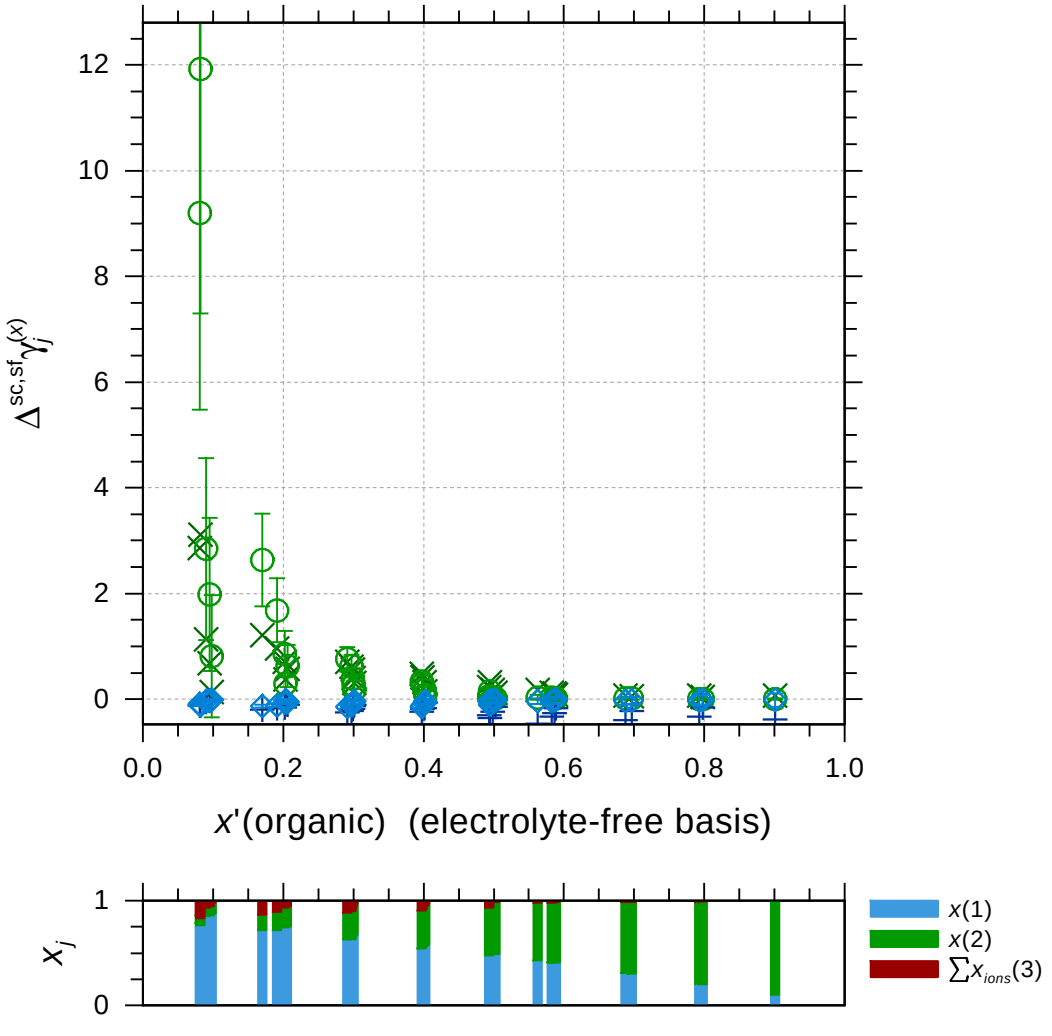
fval(0029) = 8.1216E-01

rel. contribution = 0.3862 %

Fig. S0056 (AIOMFAC_output_0030)

H_2O (1) + 1-Propanol (2) + KCl (3)

Temperature range: 361 -- 366 K

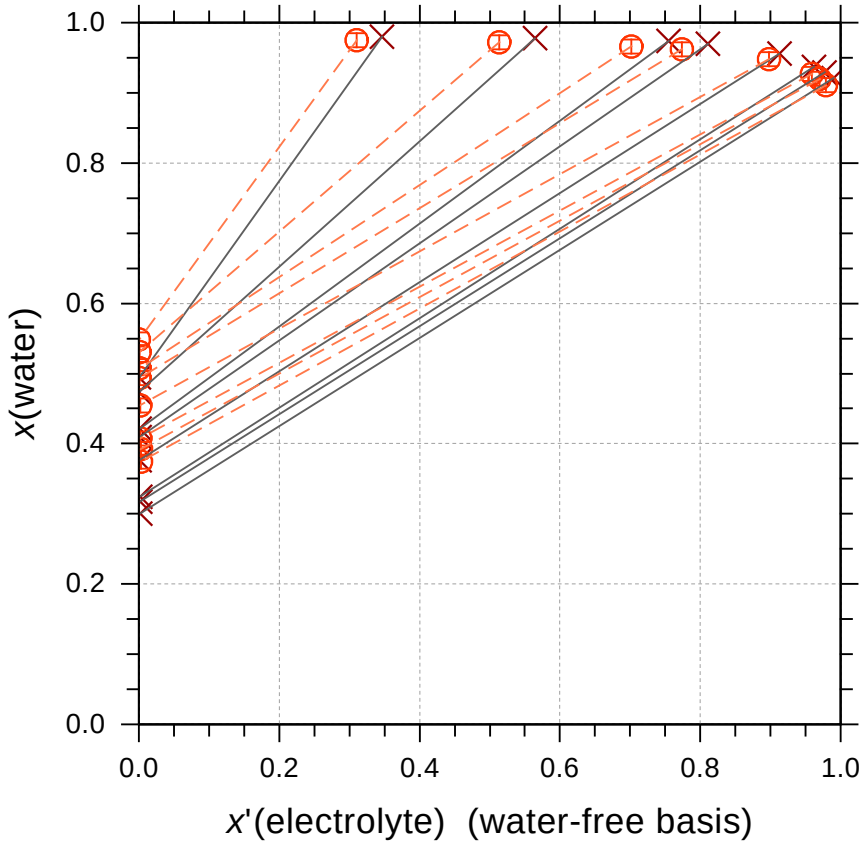


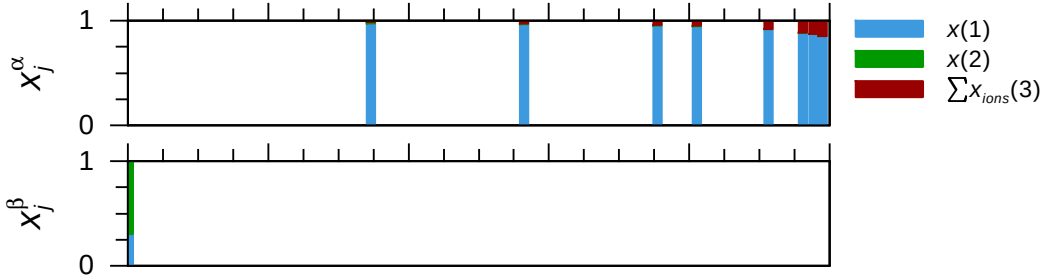
initial weighting of dataset:
$w^{init}(0030)$ = 0.500
dataset contribution to F_{obj}:
fval(0030) = 4.9600E-01
rel. contribution = 0.2359 %

Fig. S0057 (AIOMFAC_output_0031)

H_2O (1) + 1-Butanol (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl_1-BuOH_LLE_Li

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0031) = 1.000

dataset contribution to F_{obj}:

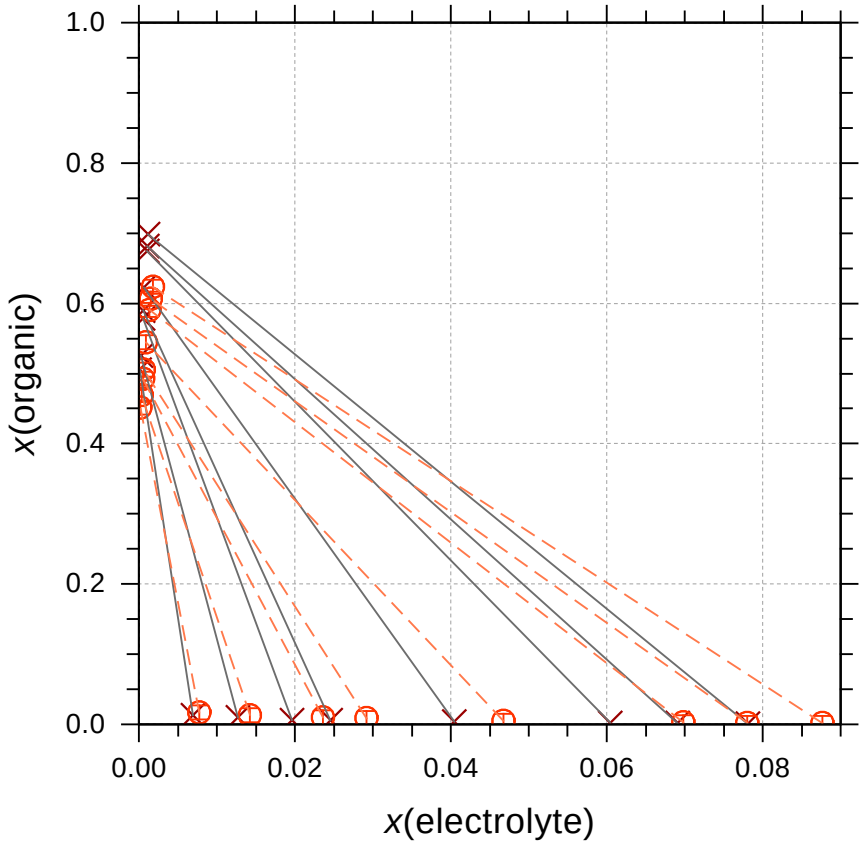
fval(0031) = 1.5419E-01

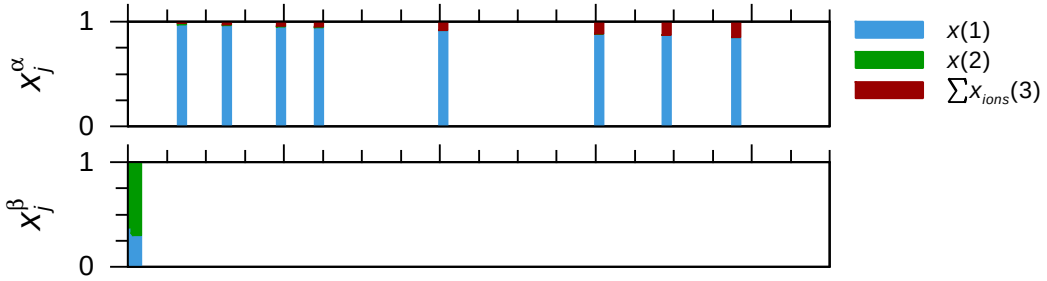
rel. contribution = 0.0733 %

Fig. S0057a (AIOMFAC_output_0031)

H_2O (1) + 1-Butanol (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl_1-BuOH_LLE_Li

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0031) = 1.000

dataset contribution to F_{obj}:

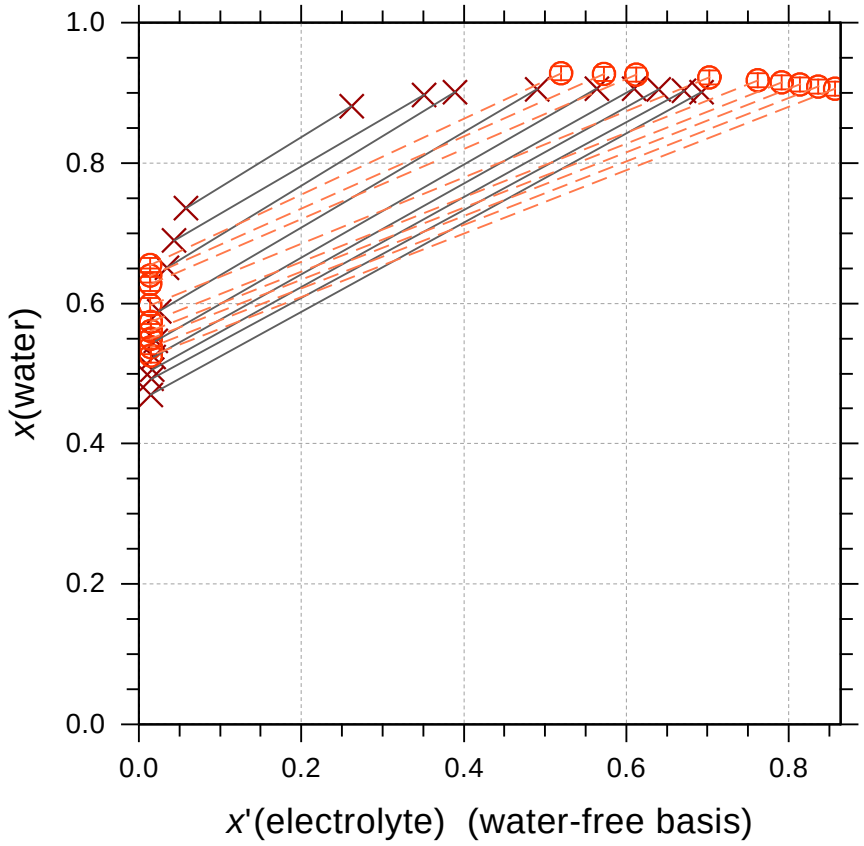
fval(0031) = 1.5419E-01

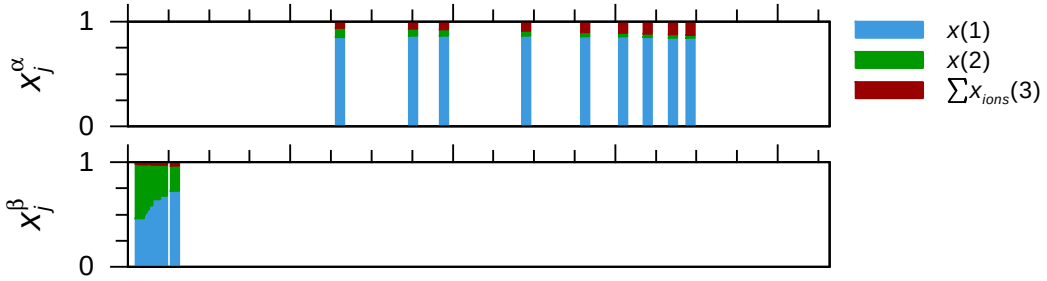
rel. contribution = 0.0733 %

Fig. S0058 (AIOMFAC_output_0041)

H_2O (1) + 1-Propanol (2) + KCl (3)

Temperature: 298 K



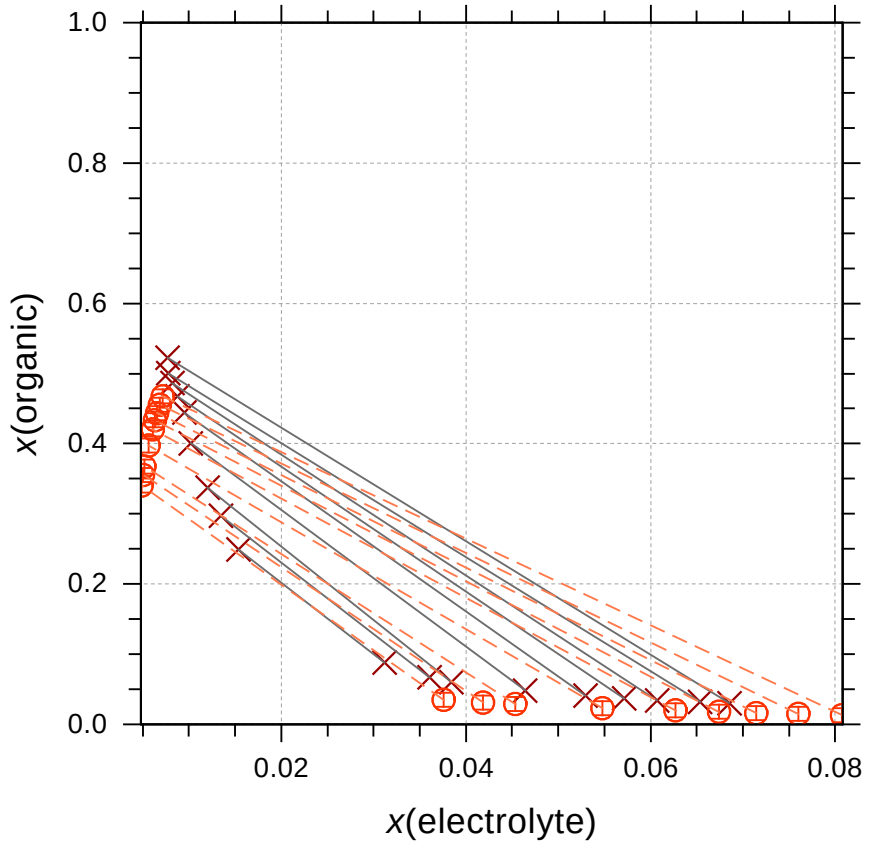


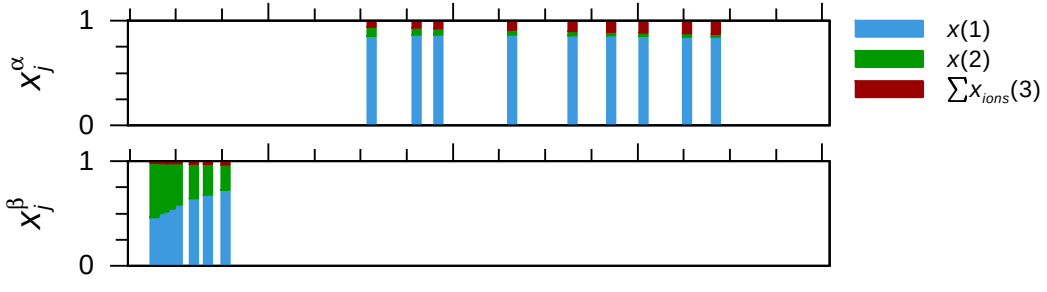
initial weighting of dataset:
$w^{init}(0041)$ = 1.000
dataset contribution to F_{obj}:
fval(0041) = 3.7646E-01
rel. contribution = 0.1790 %

Fig. S0058a (AIOMFAC_output_0041)

H_2O (1) + 1-Propanol (2) + KCl (3)

Temperature: 298 K



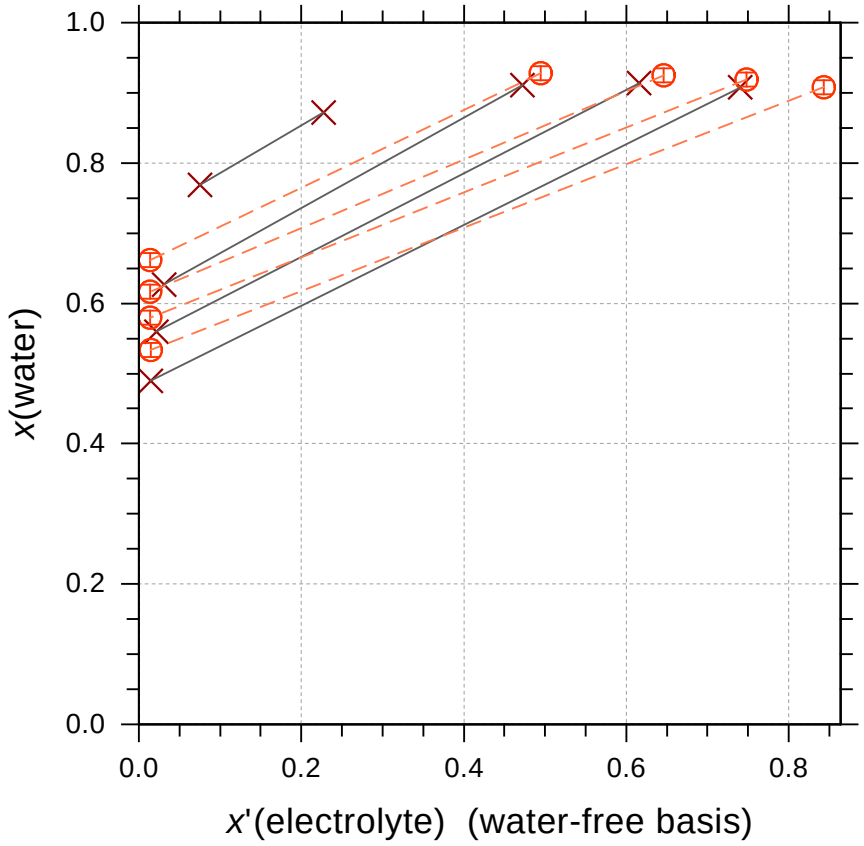


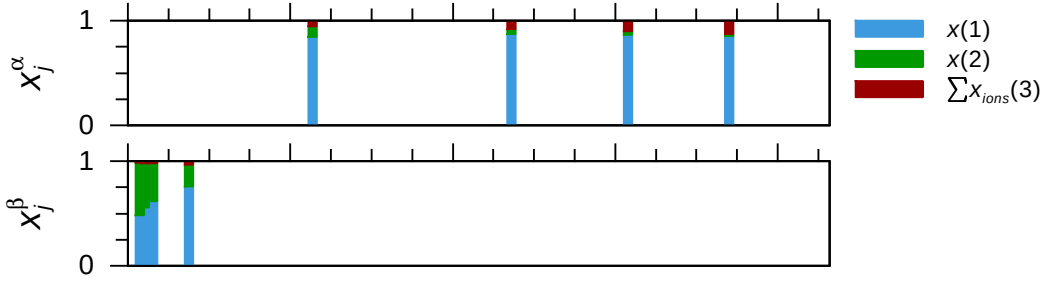
initial weighting of dataset:
w^{init}(0041) = 1.000
dataset contribution to F_{obj}:
fval(0041) = 3.7646E-01
rel. contribution = 0.1790 %

Fig. S0059 (AIOMFAC_output_0042)

H_2O (1) + 1-Propanol (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl_1-PrOH_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0042) = 1.000

dataset contribution to F_{obj}:

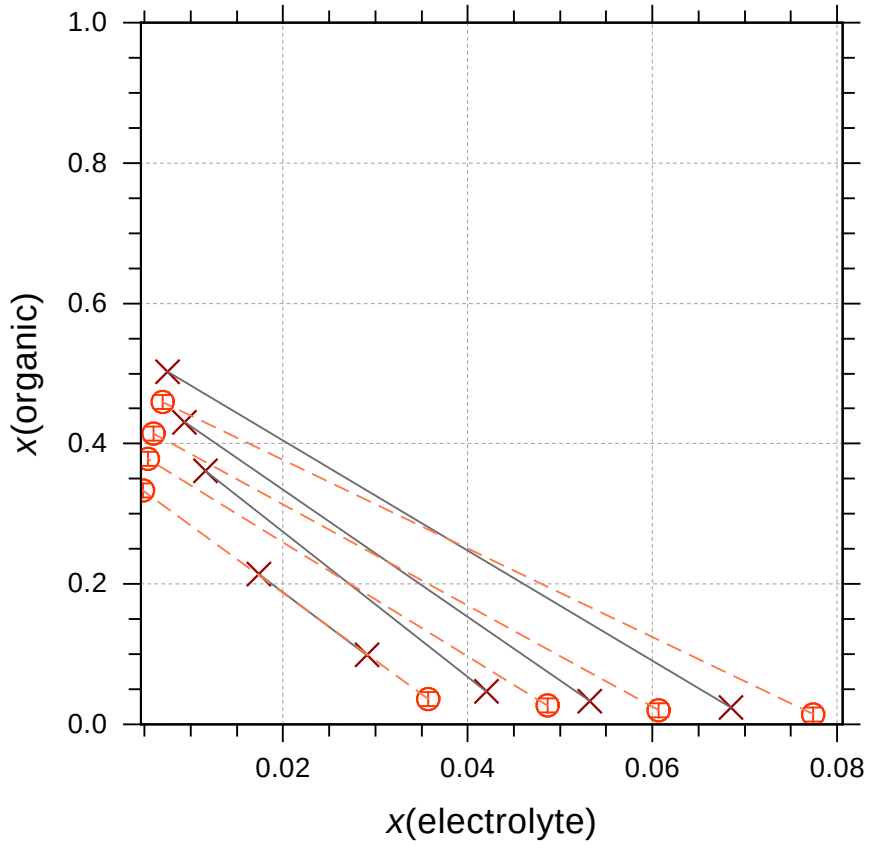
fval(0042) = 2.5738E-01

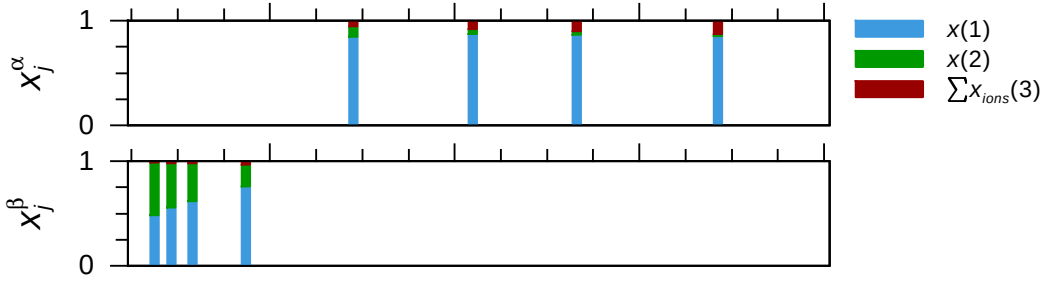
rel. contribution = 0.1224 %

Fig. S0059a (AIOMFAC_output_0042)

H_2O (1) + 1-Propanol (2) + KCl (3)

Temperature: 298 K





initial weighting of dataset:
w^{init}(0042) = 1.000
dataset contribution to F_{obj}:
fval(0042) = 2.5738E-01
rel. contribution = 0.1224 %

Fig. S0060 (AIOMFAC_output_0043)

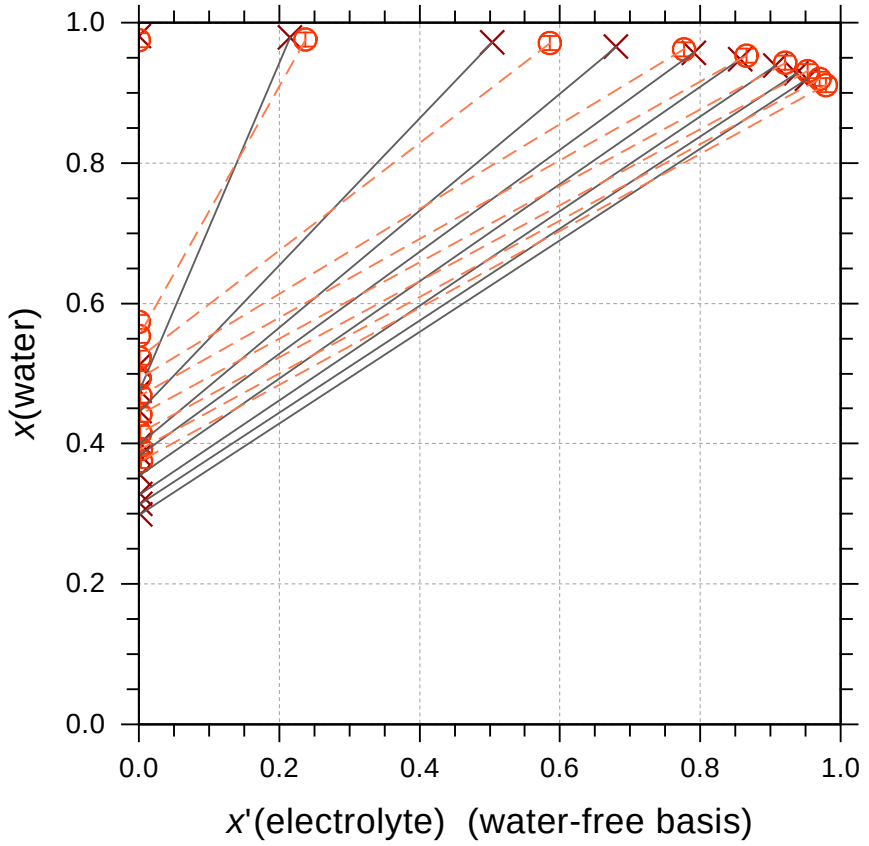
H_2O (1) + 1-Butanol (2) + KCl (3)

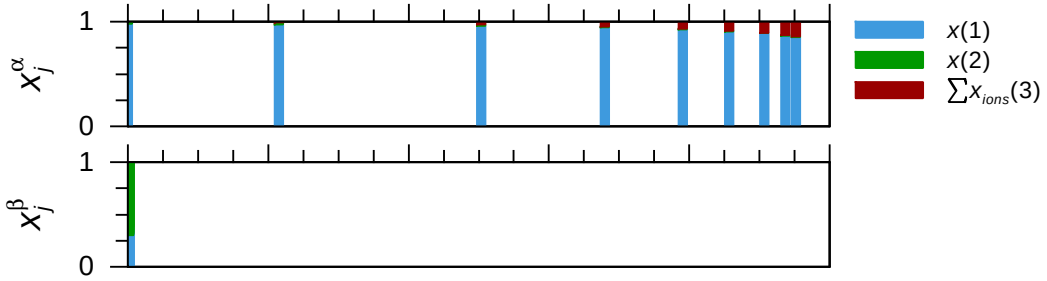
Temperature: 298 K

left y-axis:

× KCl_1-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0043) = 1.000

dataset contribution to F_{obj}:

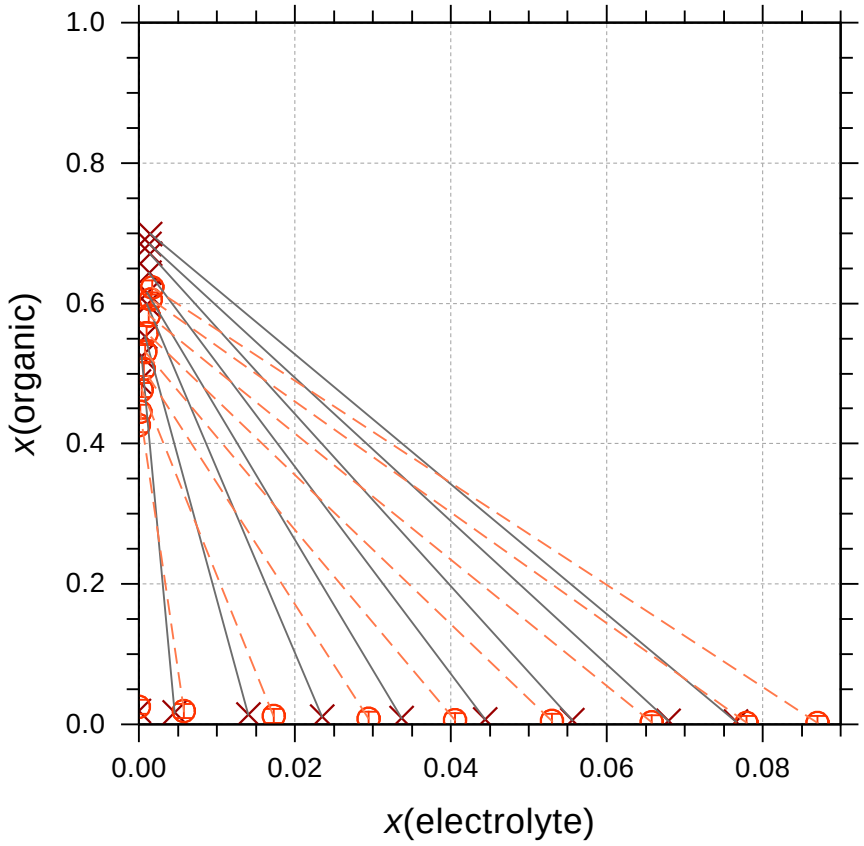
fval(0043) = 7.6736E-02

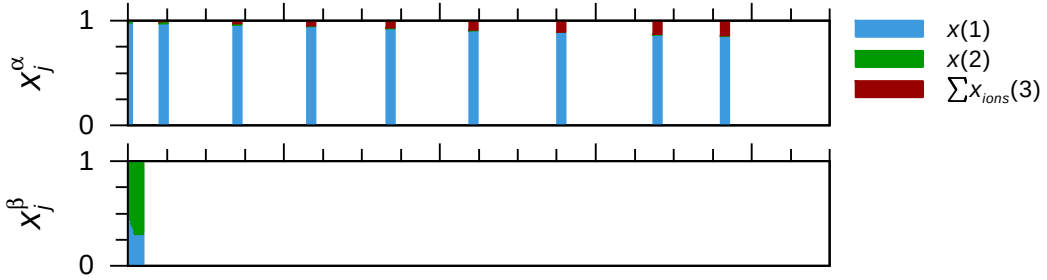
rel. contribution = 0.0365 %

Fig. S0060a (AIOMFAC_output_0043)

H_2O (1) + 1-Butanol (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl_1-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0043) = 1.000

dataset contribution to F_{obj}:

fval(0043) = 7.6736E-02

rel. contribution = 0.0365 %

Fig. S0061 (AIOMFAC_output_0044)

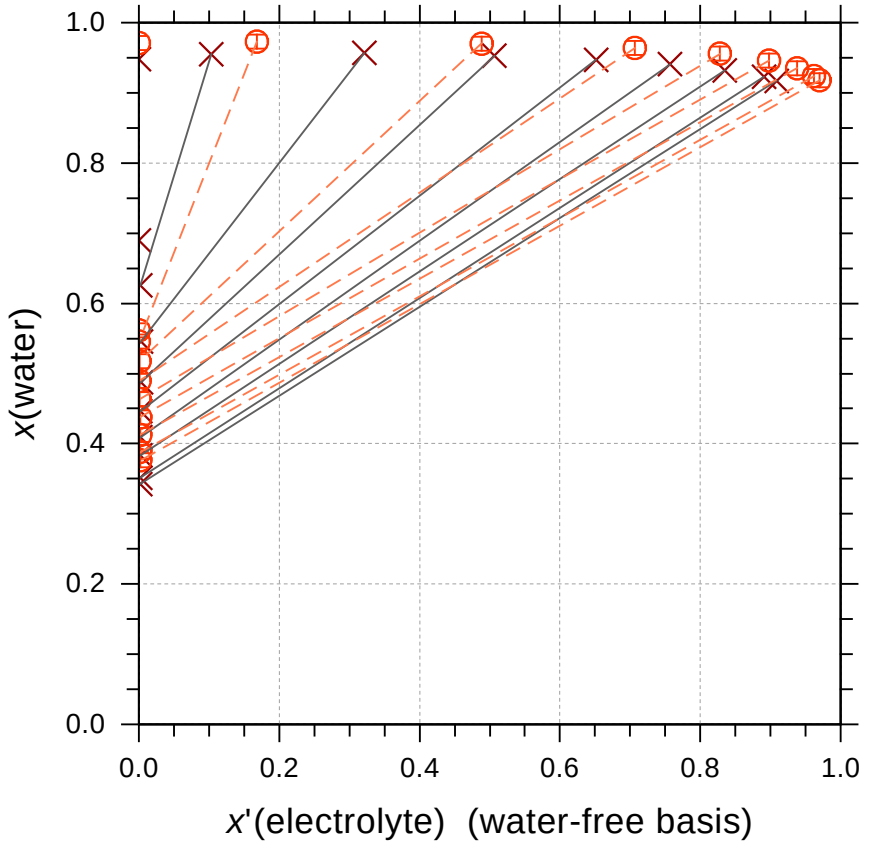
H_2O (1) + 2-Butanol (2) + KCl (3)

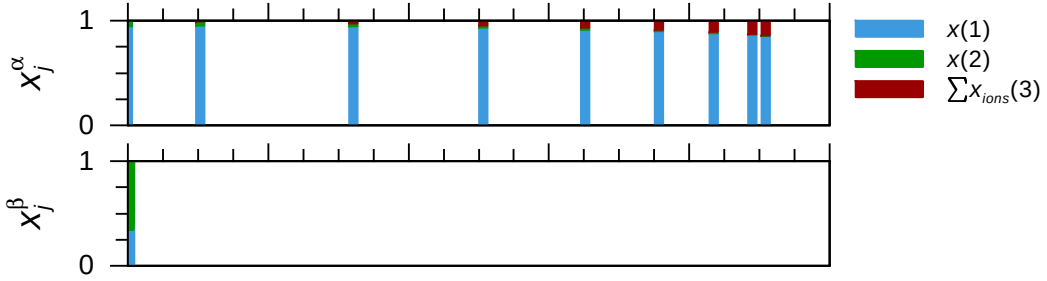
Temperature: 298 K

left y-axis:

× KCl_2-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0044) = 1.000

dataset contribution to F_{obj}:

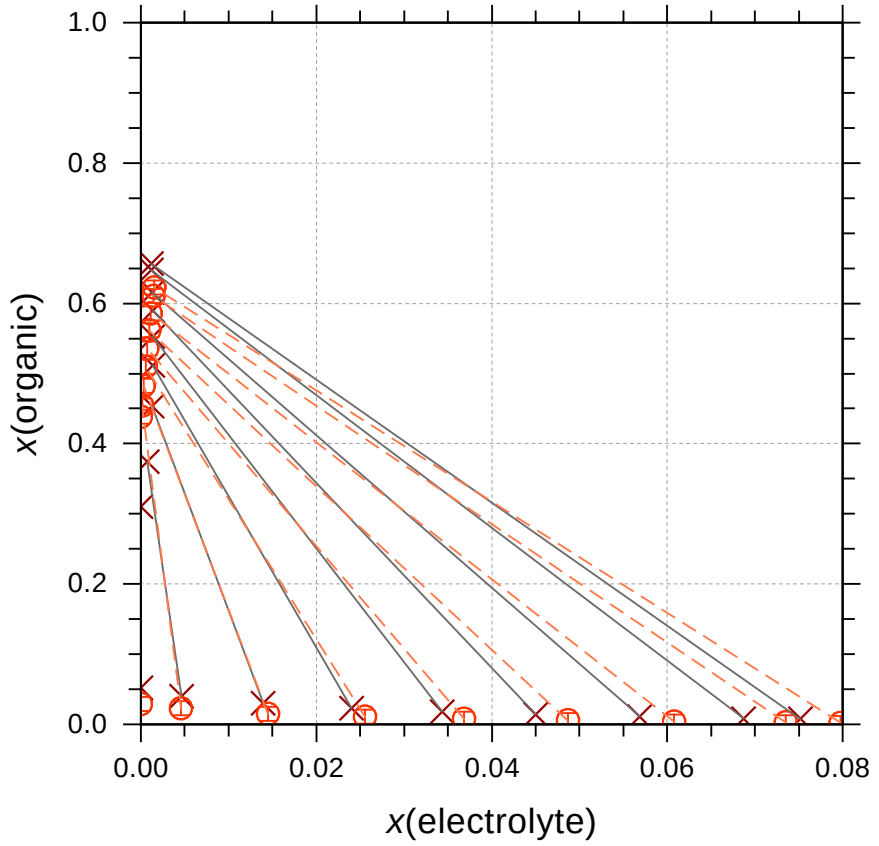
fval(0044) = 4.9945E-01

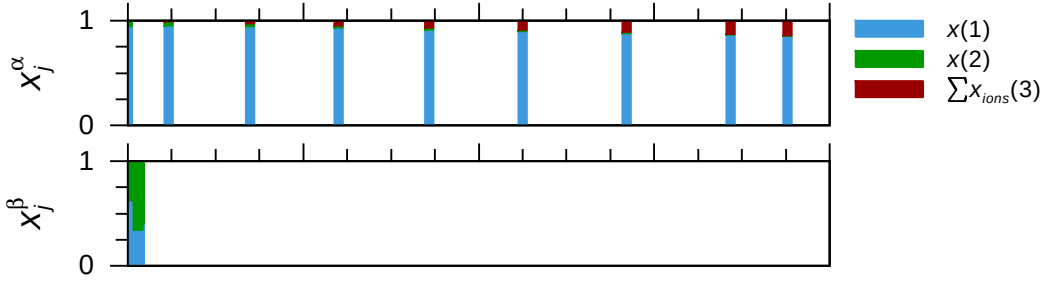
rel. contribution = 0.2375 %

Fig. S0061a (AIOMFAC_output_0044)

H_2O (1) + 2-Butanol (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl_2-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0044) = 1.000

dataset contribution to F_{obj}:

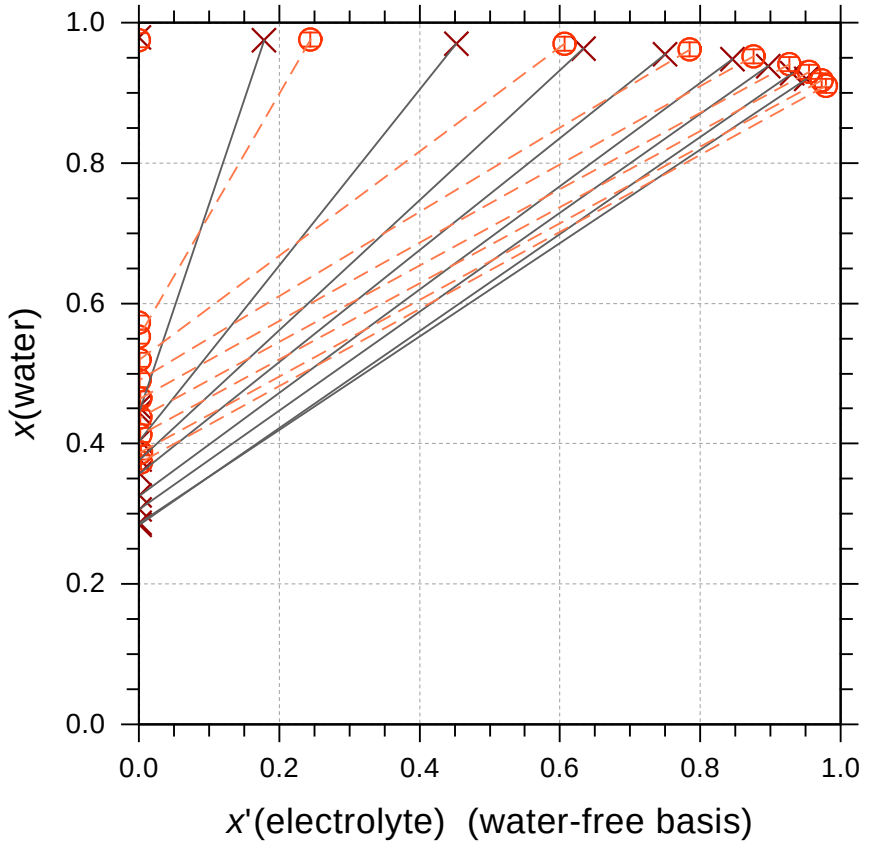
fval(0044) = 4.9945E-01

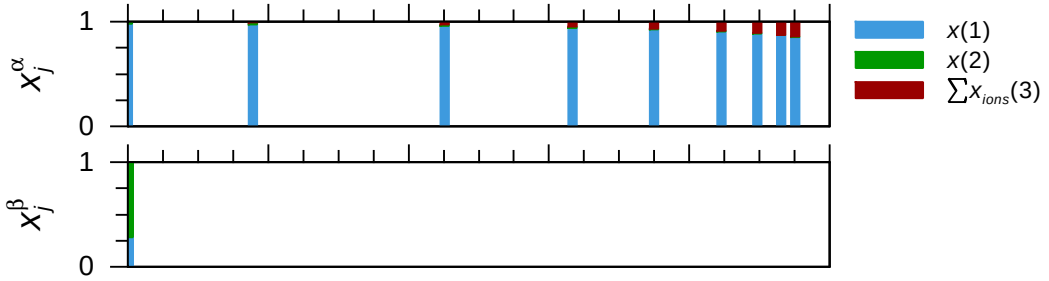
rel. contribution = 0.2375 %

Fig. S0062 (AIOMFAC_output_0045)

H_2O (1) + Isobutanol (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl_iso-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0045) = 1.000

dataset contribution to F_{obj}:

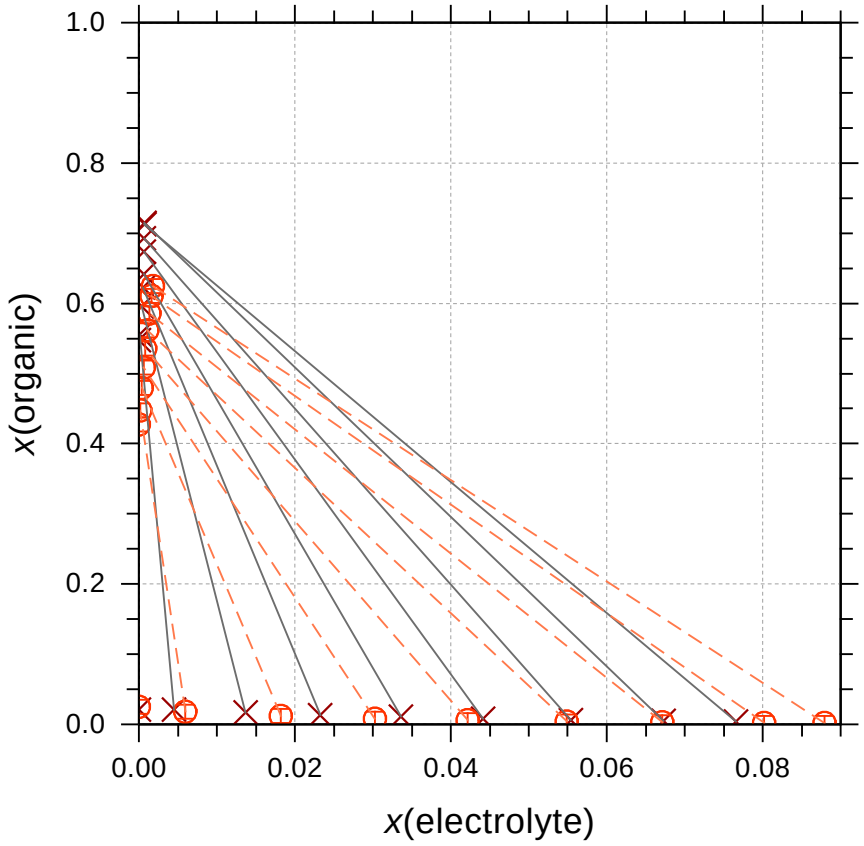
fval(0045) = 1.0972E-01

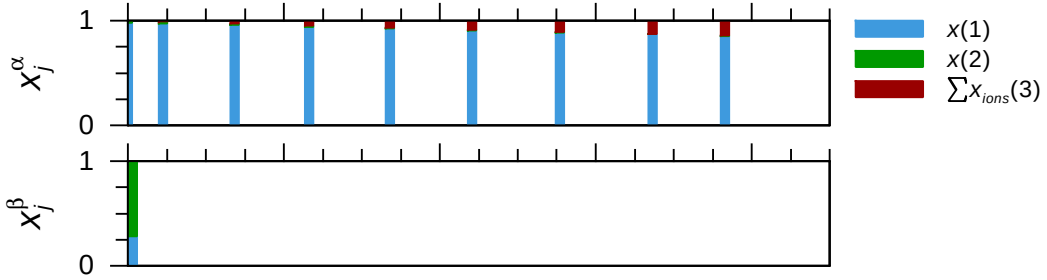
rel. contribution = 0.0522 %

Fig. S0062a (AIOMFAC_output_0045)

H_2O (1) + Isobutanol (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl_iso-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0045) = 1.000

dataset contribution to F_{obj}:

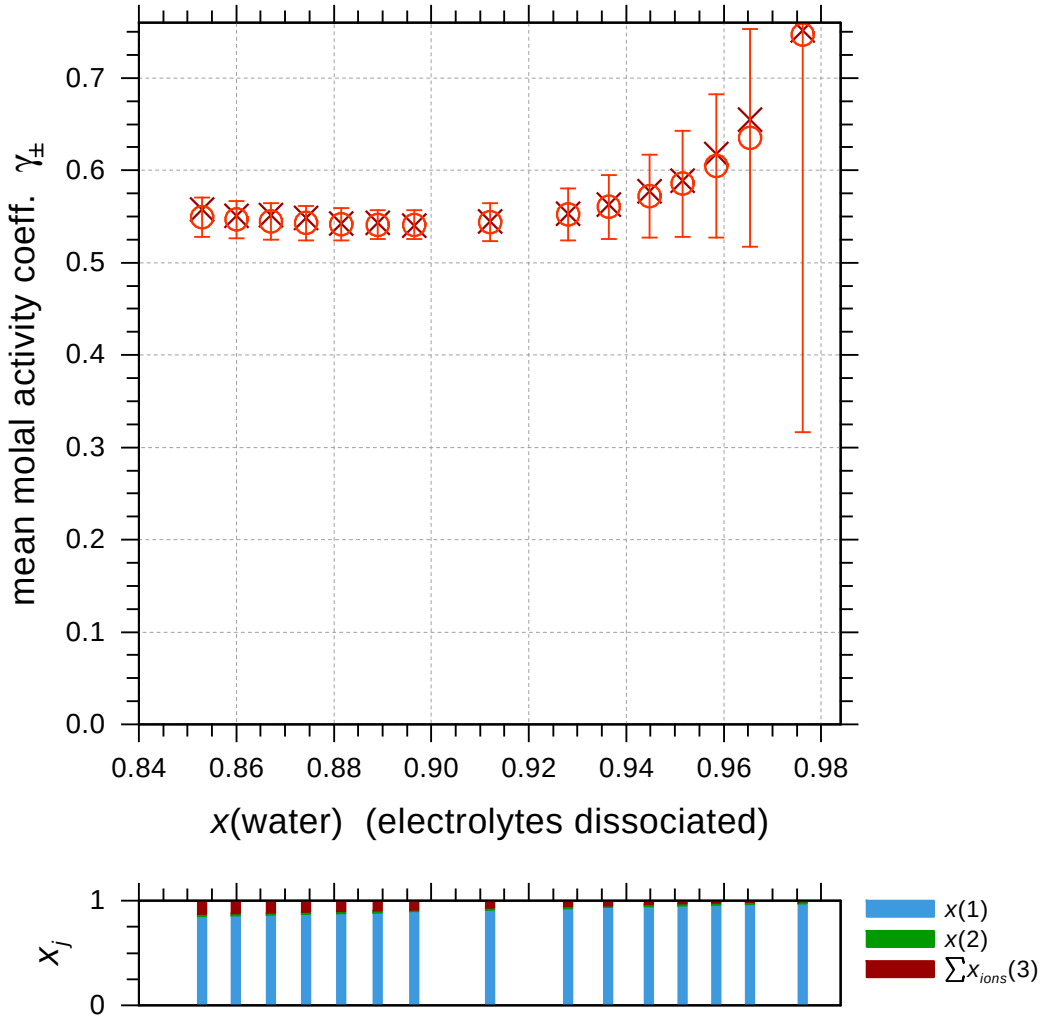
fval(0045) = 1.0972E-01

rel. contribution = 0.0522 %

Fig. S0063 (AIOMFAC_output_0112)

H_2O (1) + Ethanol (2) + KCl (3)

Temperature: 298 K

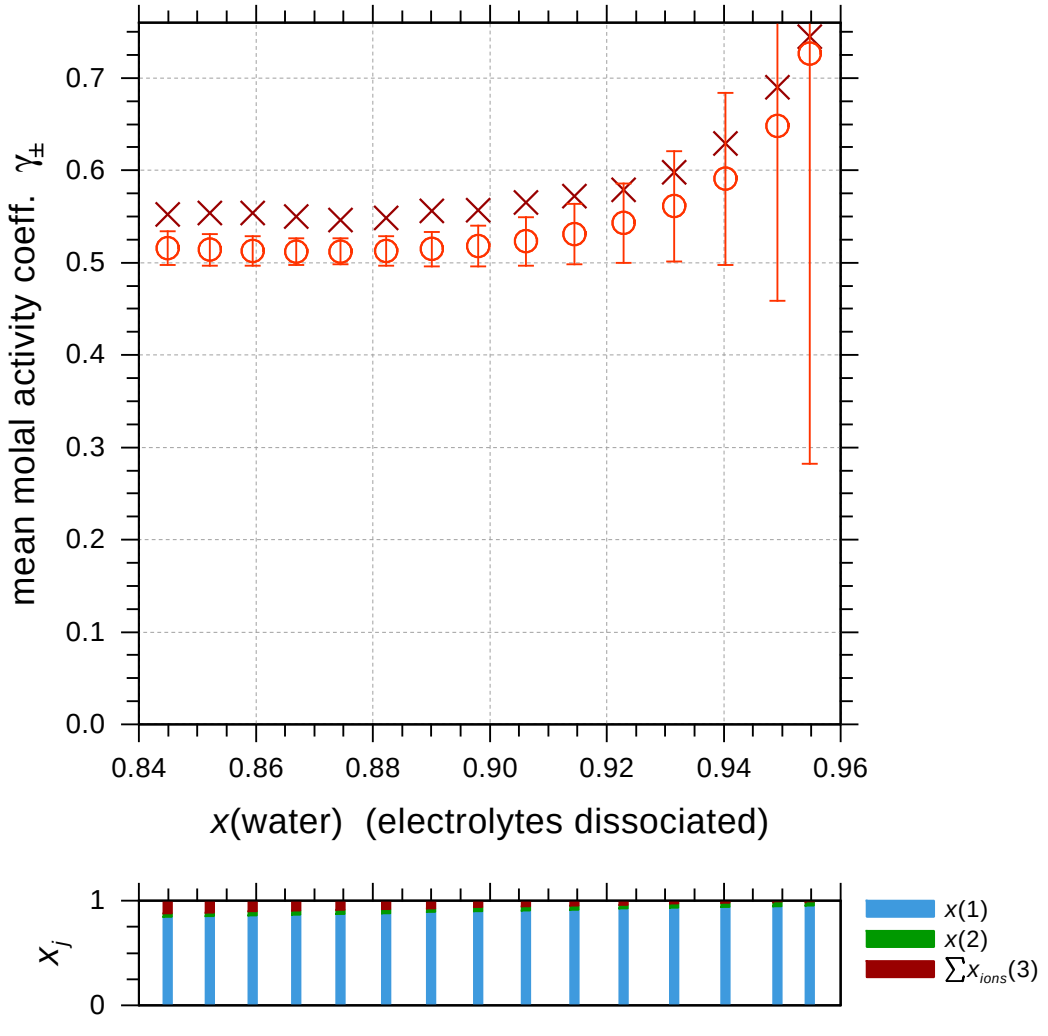


initial weighting of dataset:
$w^{init}(0112)$ = 2.000
dataset contribution to F_{obj}:
fval(0112) = 2.2463E-03
rel. contribution = 0.0011 %

Fig. S0064 (AIOMFAC_output_0113)

H_2O (1) + Ethanol (2) + KCl (3)

Temperature: 298 K

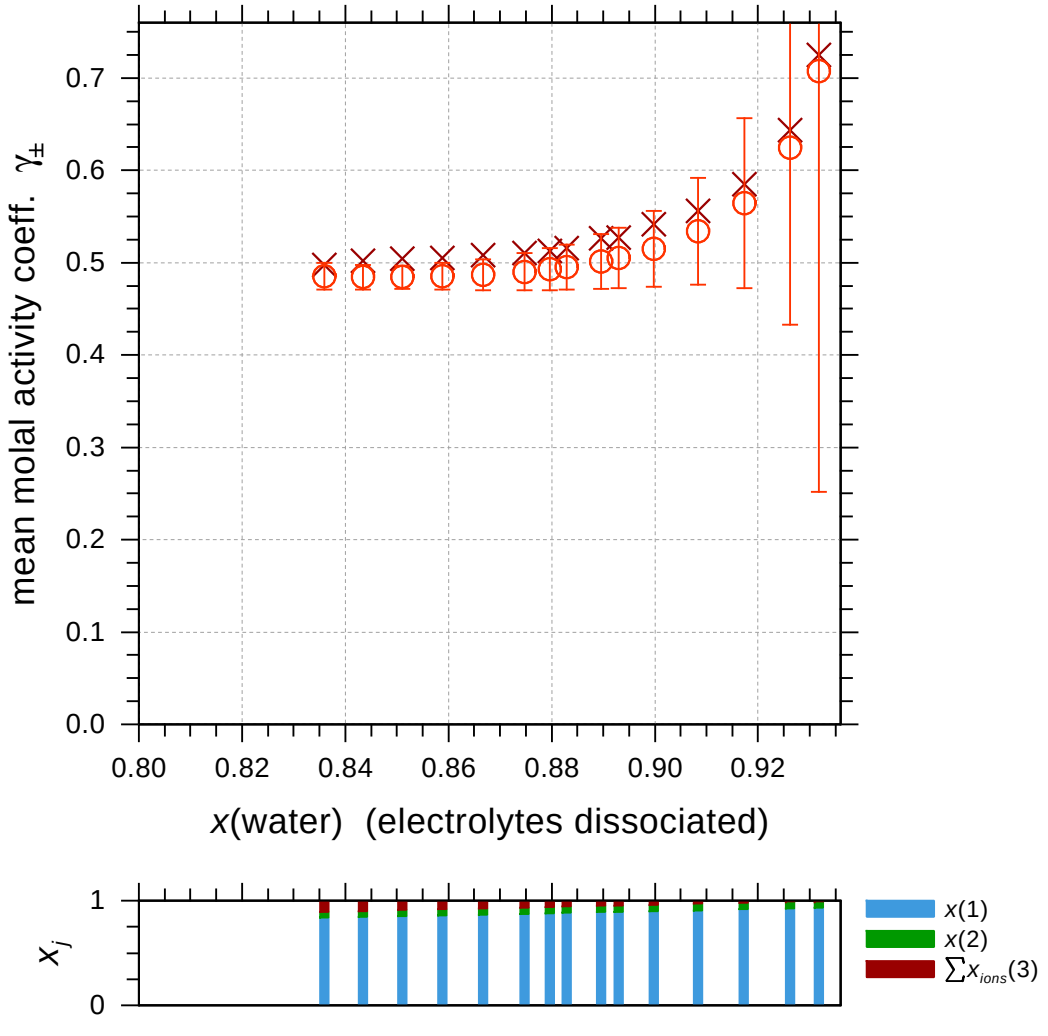


initial weighting of dataset:
$w^{init}(0113)$ = 2.000
dataset contribution to F_{obj}:
fval(0113) = 7.6760E-02
rel. contribution = 0.0365 %

Fig. S0065 (AIOMFAC_output_0114)

H_2O (1) + Ethanol (2) + KCl (3)

Temperature: 298 K

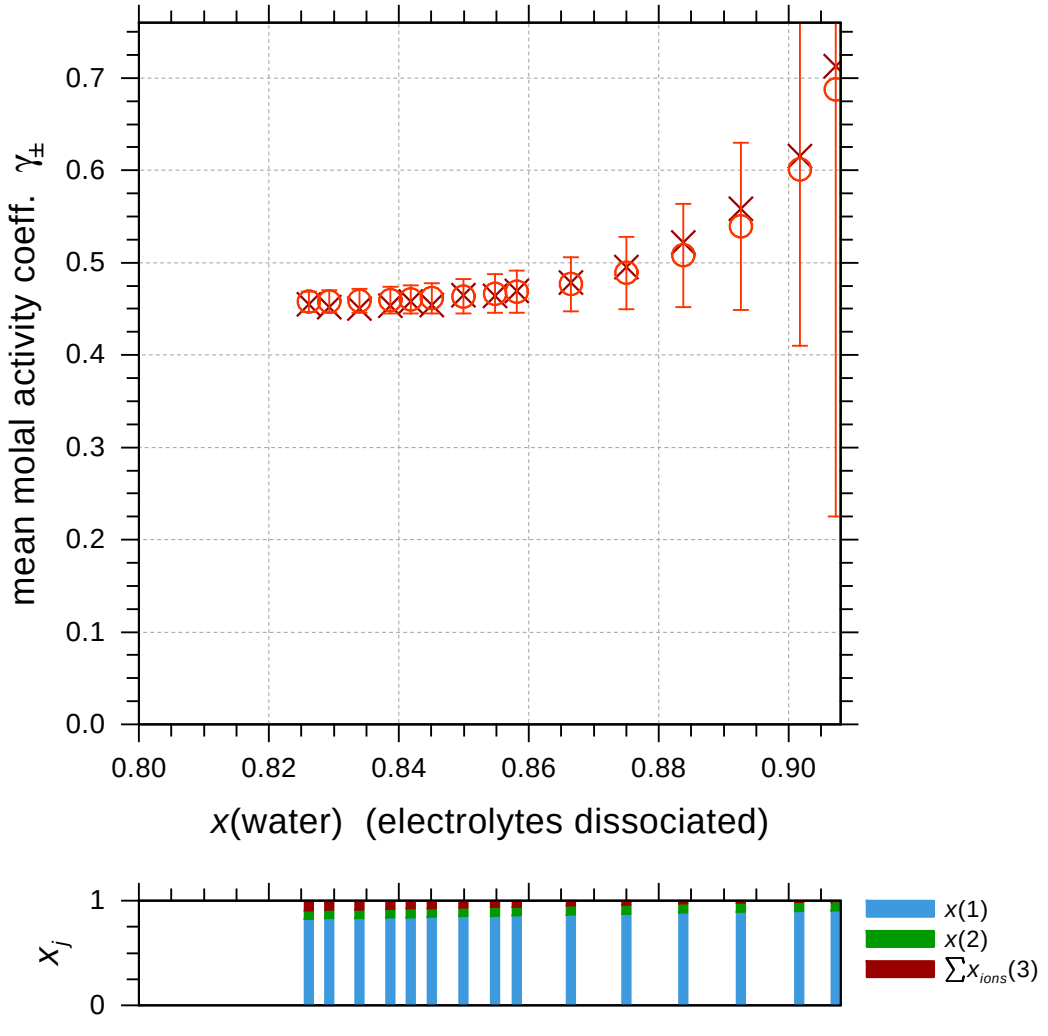


initial weighting of dataset:
$w^{init}(0114)$ = 2.000
dataset contribution to F_{obj}:
fval(0114) = 2.5692E-02
rel. contribution = 0.0122 %

Fig. S0066 (AIOMFAC_output_0115)

H_2O (1) + Ethanol (2) + KCl (3)

Temperature: 298 K



initial weighting of dataset:
$w^{init}(0115)$ = 2.000
dataset contribution to F_{obj}:
fval(0115) = 4.4531E-03
rel. contribution = 0.0021 %

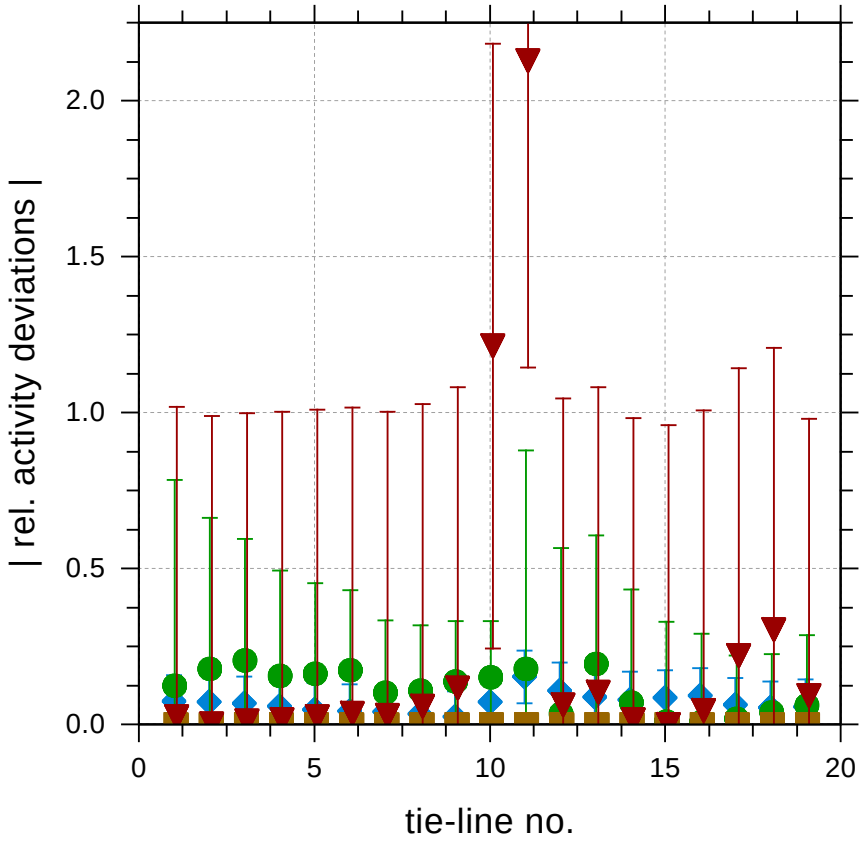
Fig. S0067 (AIOMFAC_output_1012)

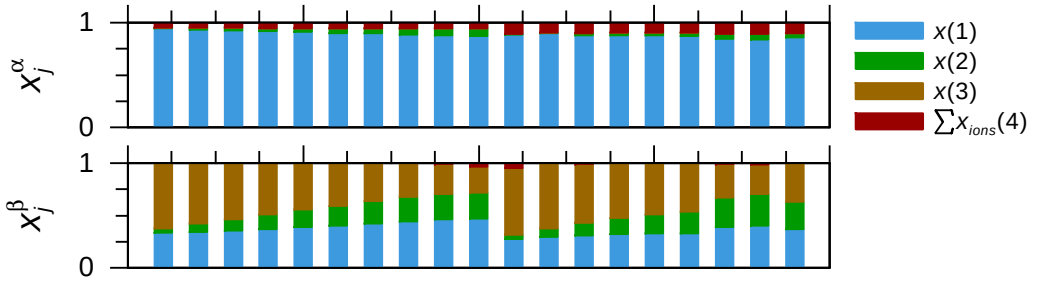
H_2O (1) + Ethanol (2) + 1-Pentanol (3) + KCl (4)

Temperature: 298 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



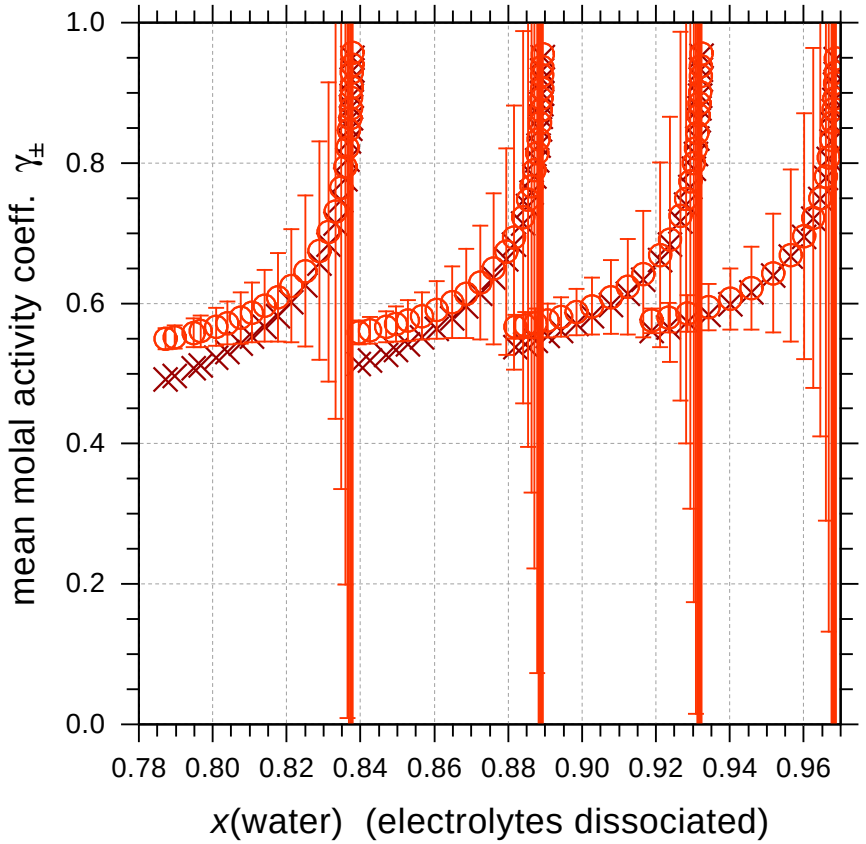


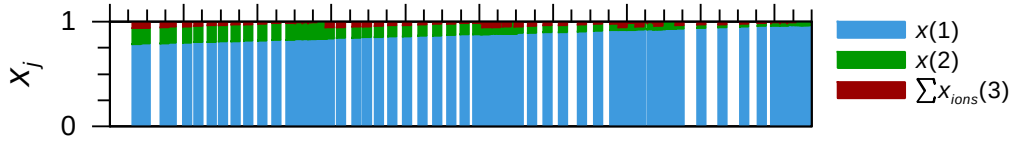
initial weighting of dataset:
$w^{init}(1012)$ = 1.000
dataset contribution to F_{obj}:
fval(1012) = 1.7398E+00
rel. contribution = 0.8273 %

Fig. S0068 (AIOMFAC_output_1046)

H_2O (1) + 1,2-Ethanediol (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl+1,2-Ethanediol+Water_EMF_Ma

○ AIOMFAC mean molal activity coeff. $\gamma_{\pm}$

initial weighting of dataset:

$w^{init}(1046)$ = 2.000

dataset contribution to F_{obj}:

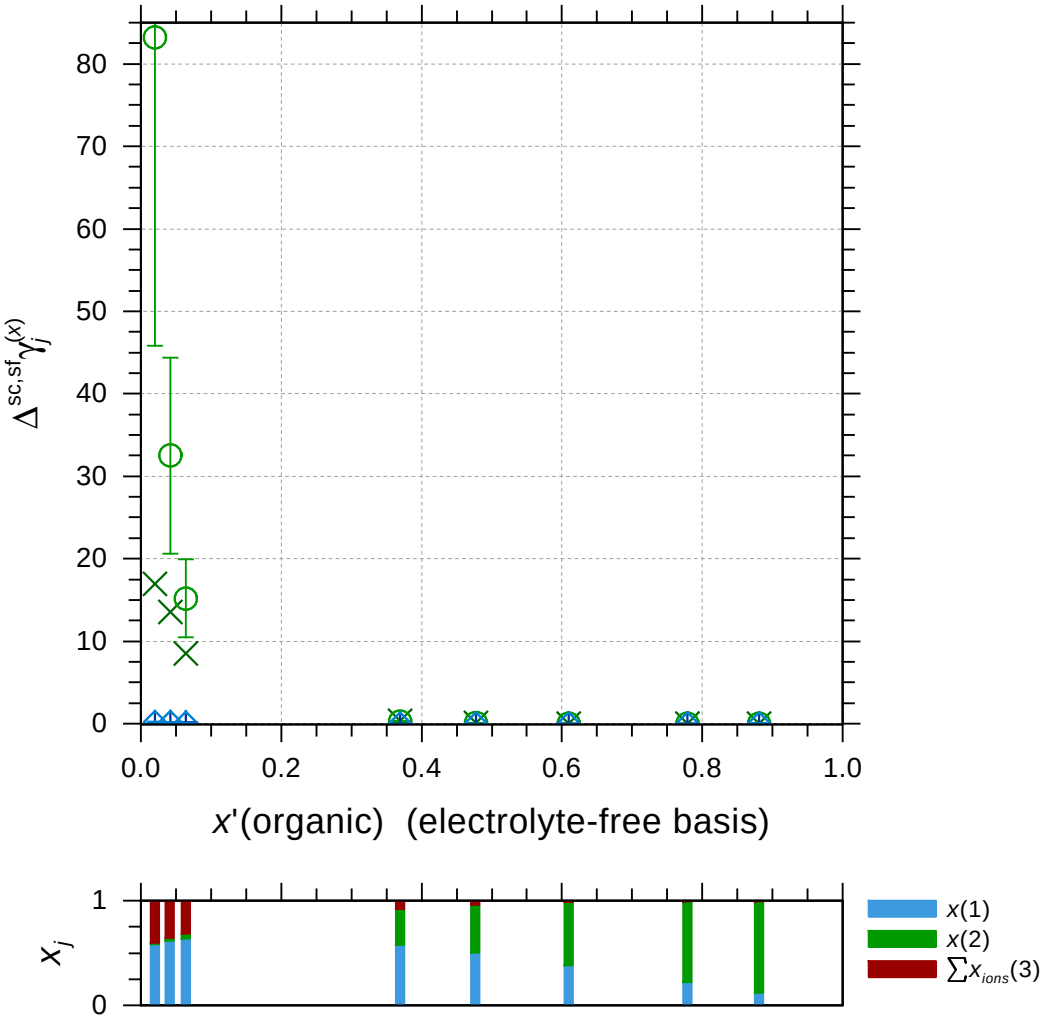
fval(1046) = 2.4810E-02

rel. contribution = 0.0118 %

Fig. S0069 (AIOMFAC_output_0069)

H_2O (1) + Ethanol (2) + KNO_3 (3)

Temperature range: 351 -- 369 K



initial weighting of dataset:

w^{init}(0069) = 0.500

dataset contribution to F_{obj}:

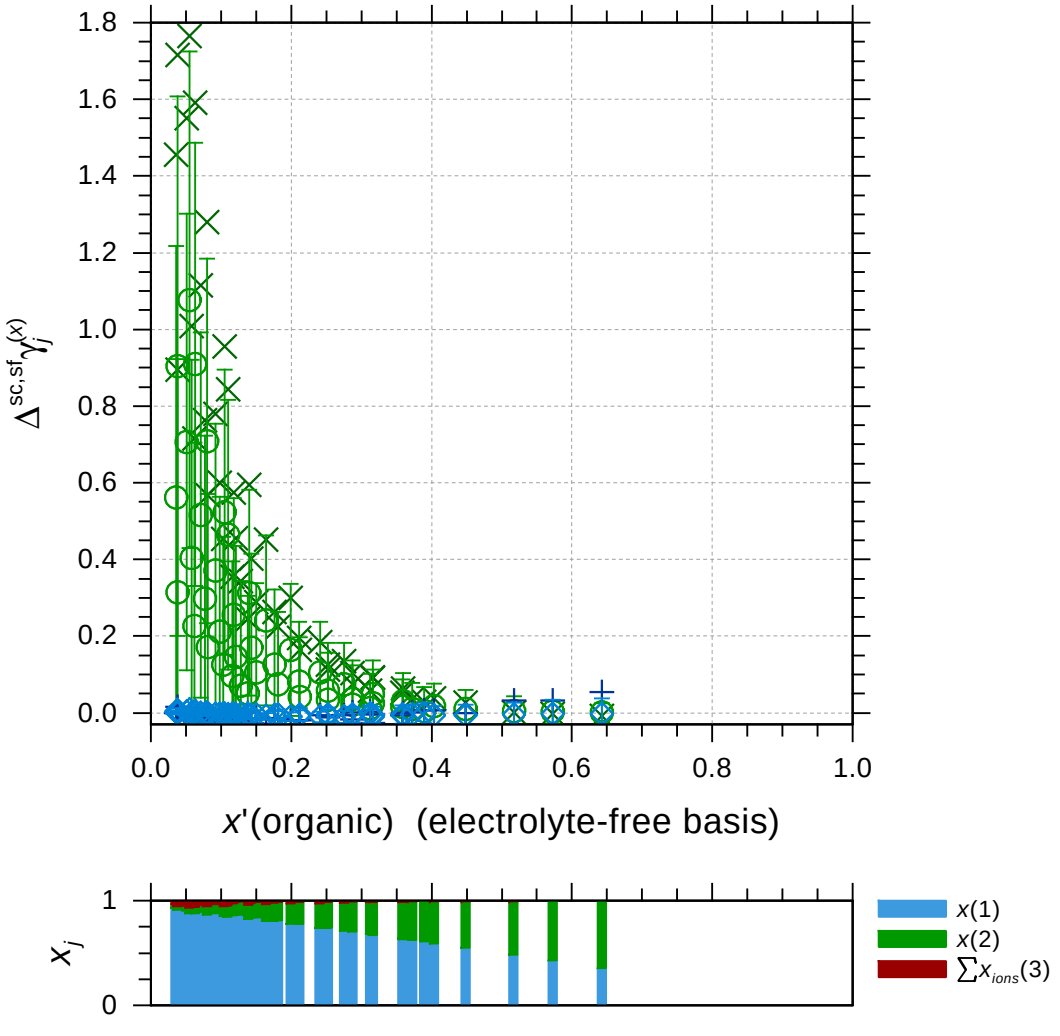
fval(0069) = 1.1199E+00

rel. contribution = 0.5325 %

Fig. S0070 (AIOMFAC_output_0070)

H_2O (1) + Ethanol (2) + KNO_3 (3)

Temperature range: 352 -- 364 K



initial weighting of dataset:

w^{init}(0070) = 0.500

dataset contribution to F_{obj}:

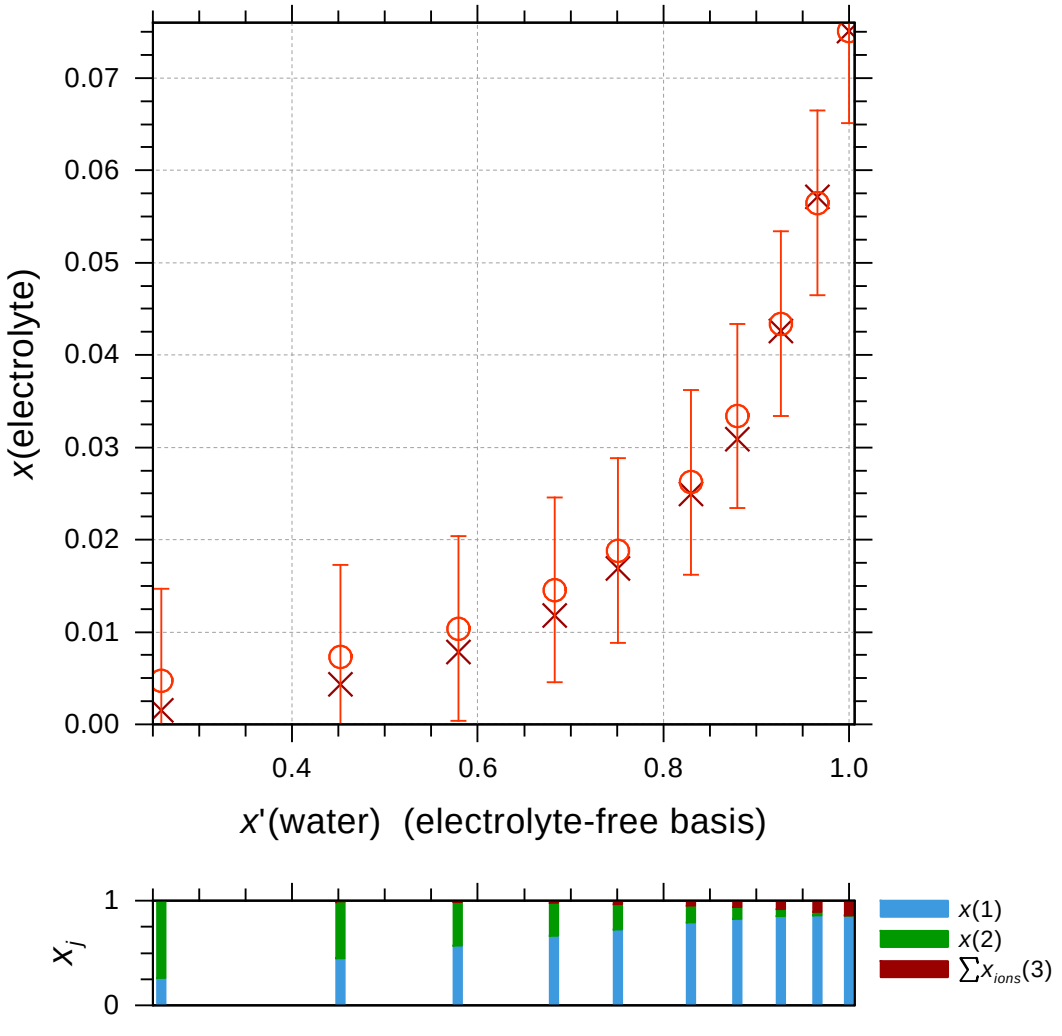
fval(0070) = 1.1252E-01

rel. contribution = 0.0535 %

Fig. S0071 (AIOMFAC_output_0071)

H_2O (1) + Ethanol (2) + KNO_3 (3)

Temperature: 303 K

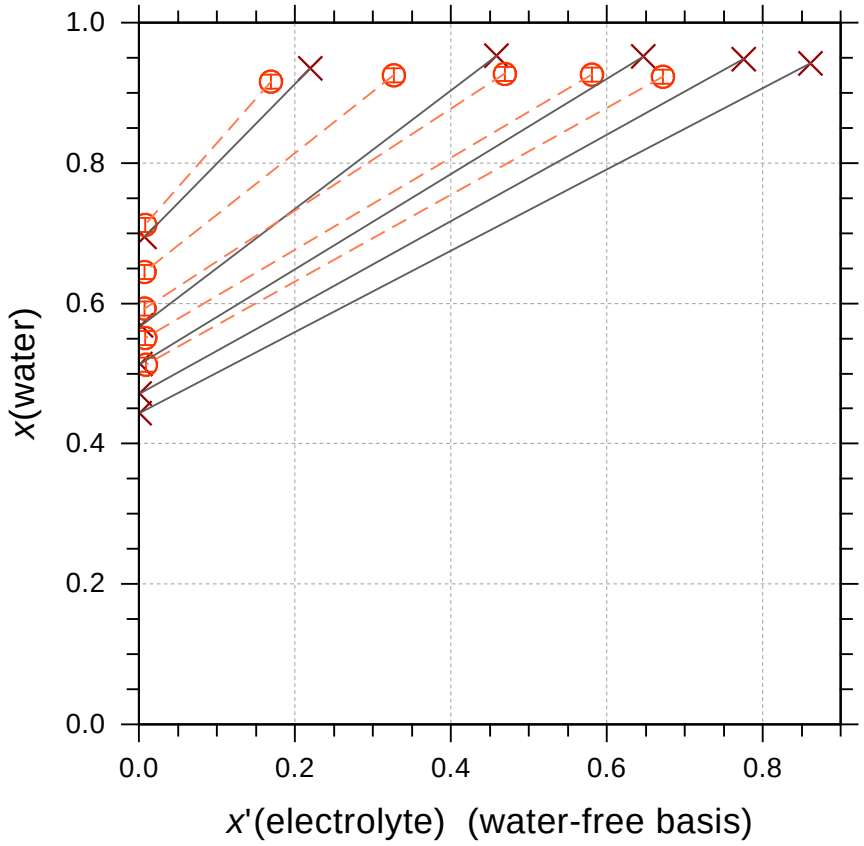


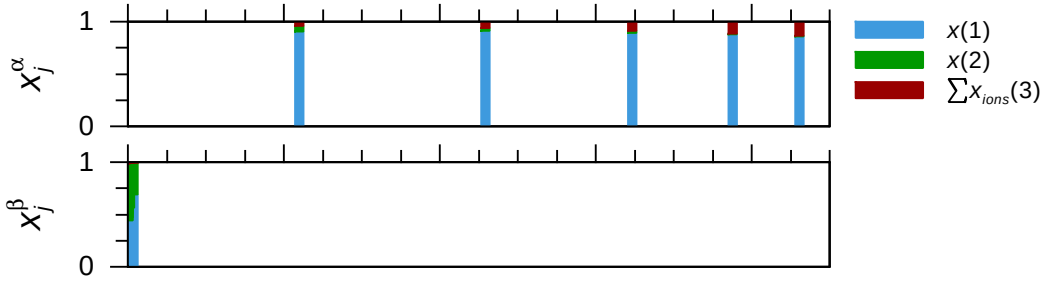
initial weighting of dataset:
$w^{init}(0071)$ = 1.000
dataset contribution to F_{obj}:
fval(0071) = 1.6386E-01
rel. contribution = 0.0779 %

Fig. S0072 (AIOMFAC_output_1066)

H_2O (1) + 1-Propanol (2) + Li_2SO_4 (3)

Temperature: 298 K





left y-axis:

× Li2SO4+1-Propanol+Water_LLE_Taboada

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1066) = 1.000

dataset contribution to F_{obj}:

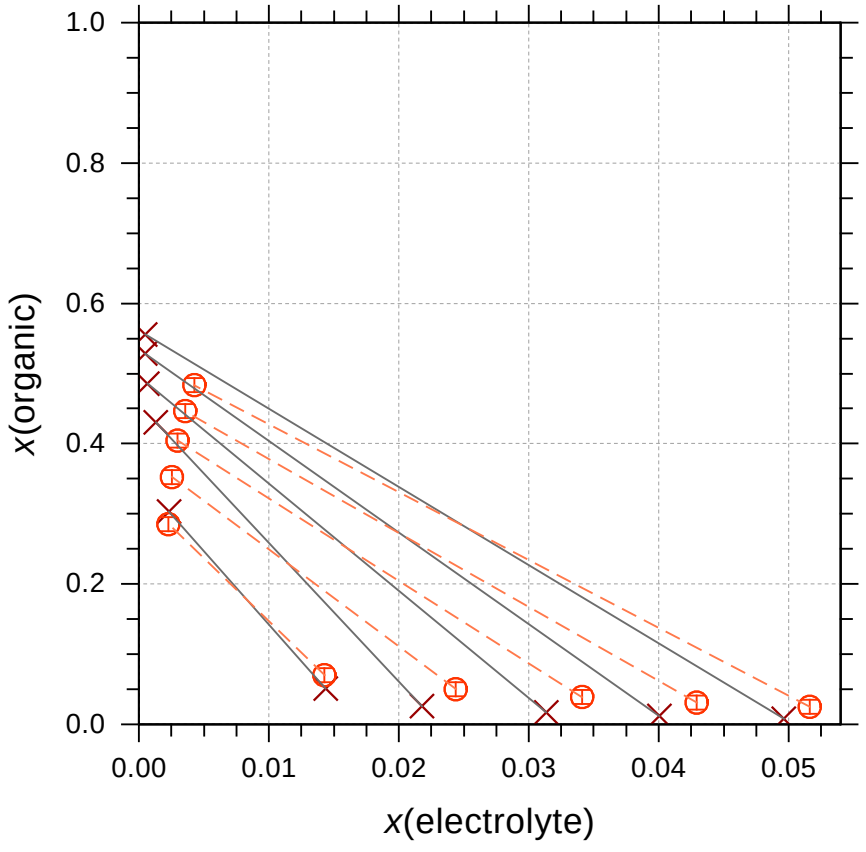
fval(1066) = 5.2082E-01

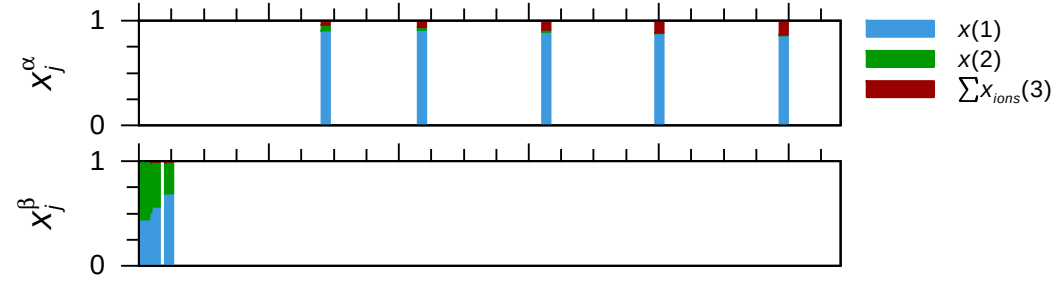
rel. contribution = 0.2477 %

Fig. S0072a (AIOMFAC_output_1066)

H_2O (1) + 1-Propanol (2) + Li_2SO_4 (3)

Temperature: 298 K



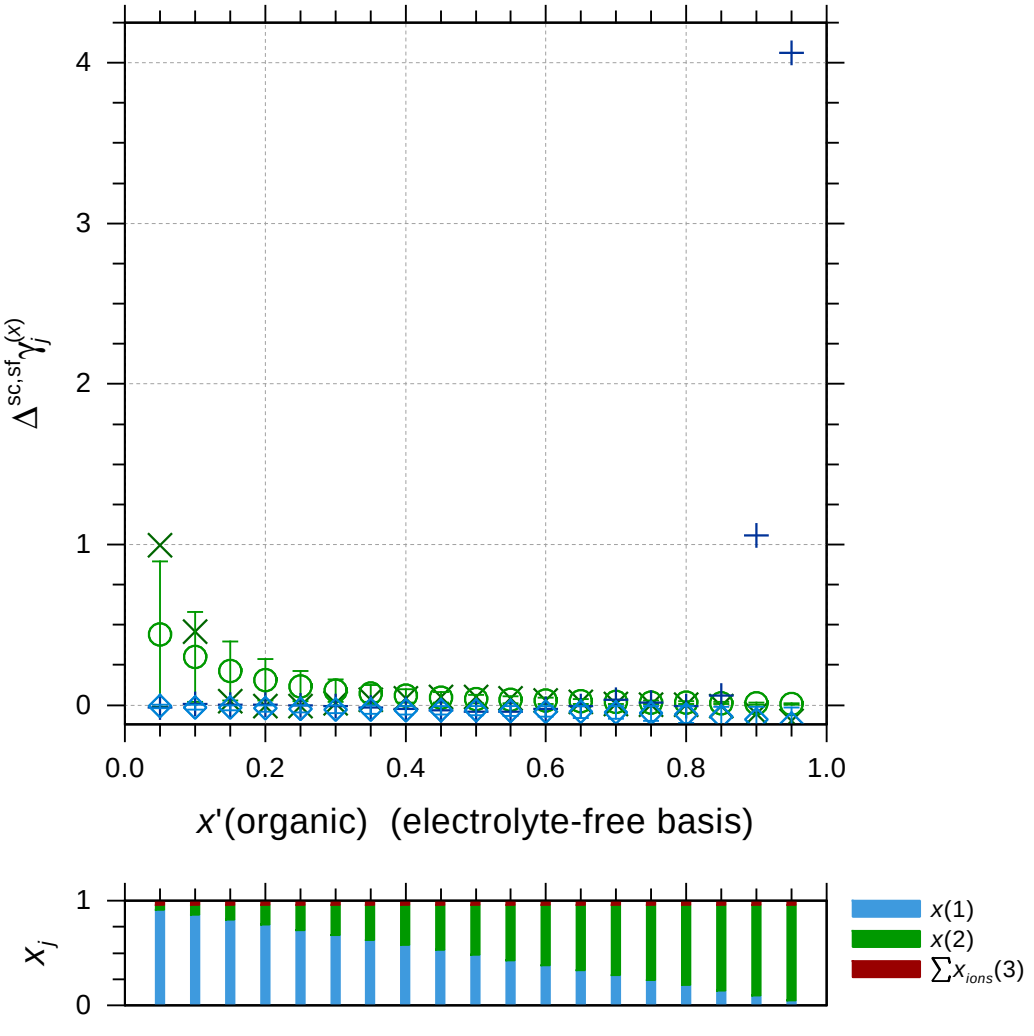


initial weighting of dataset:
w^{init}(1066) = 1.000
dataset contribution to F_{obj}:
fval(1066) = 5.2082E-01
rel. contribution = 0.2477 %

Fig. S0073 (AIOMFAC_output_0099)

H_2O (1) + Ethanol (2) + LiBr (3)

Temperature: 333 K

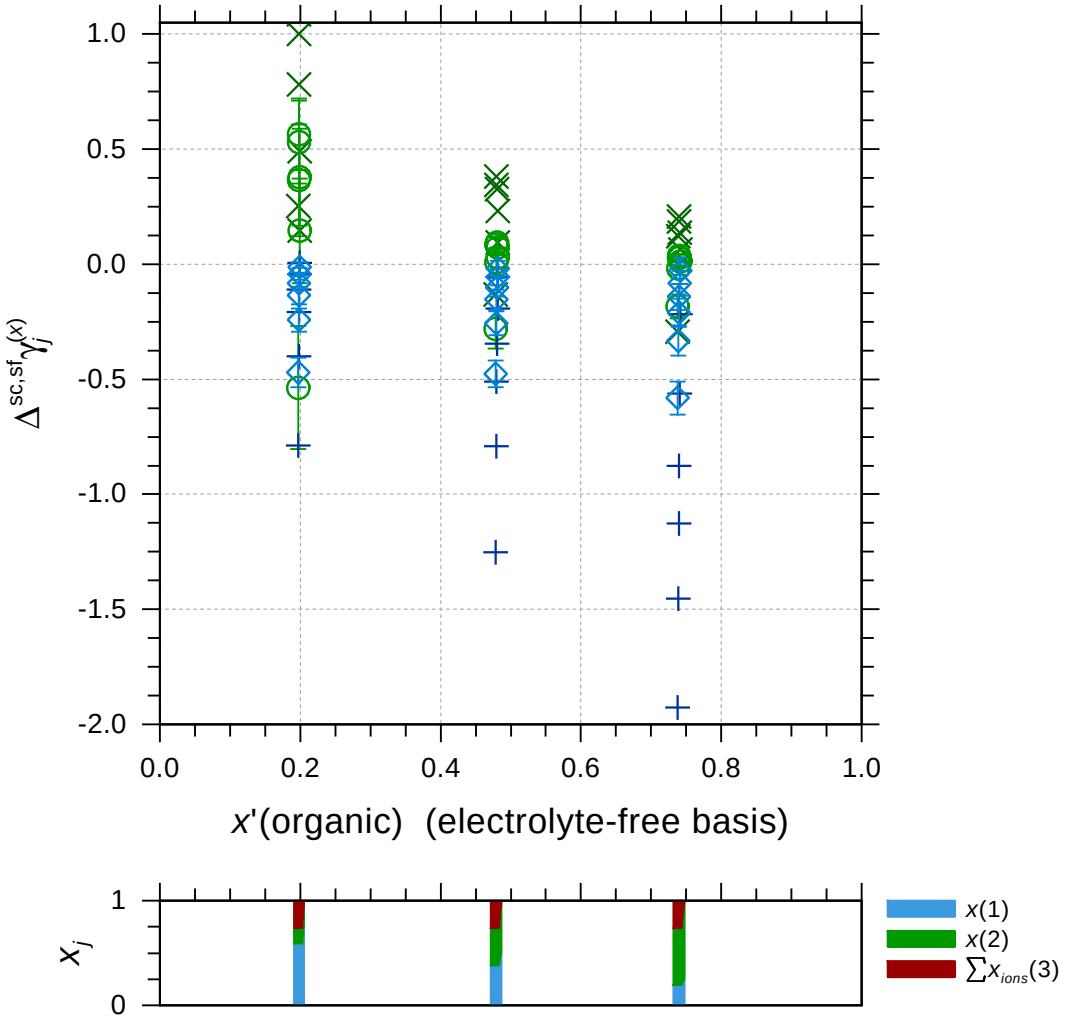


initial weighting of dataset:
$w^{init}(0099)$ = 0.050
dataset contribution to F_{obj}:
fval(0099) = 2.9238E-02
rel. contribution = 0.0139 %

Fig. S0074 (AIOMFAC_output_0100)

H_2O (1) + 2-Propanol (2) + LiBr (3)

Temperature: 348 K

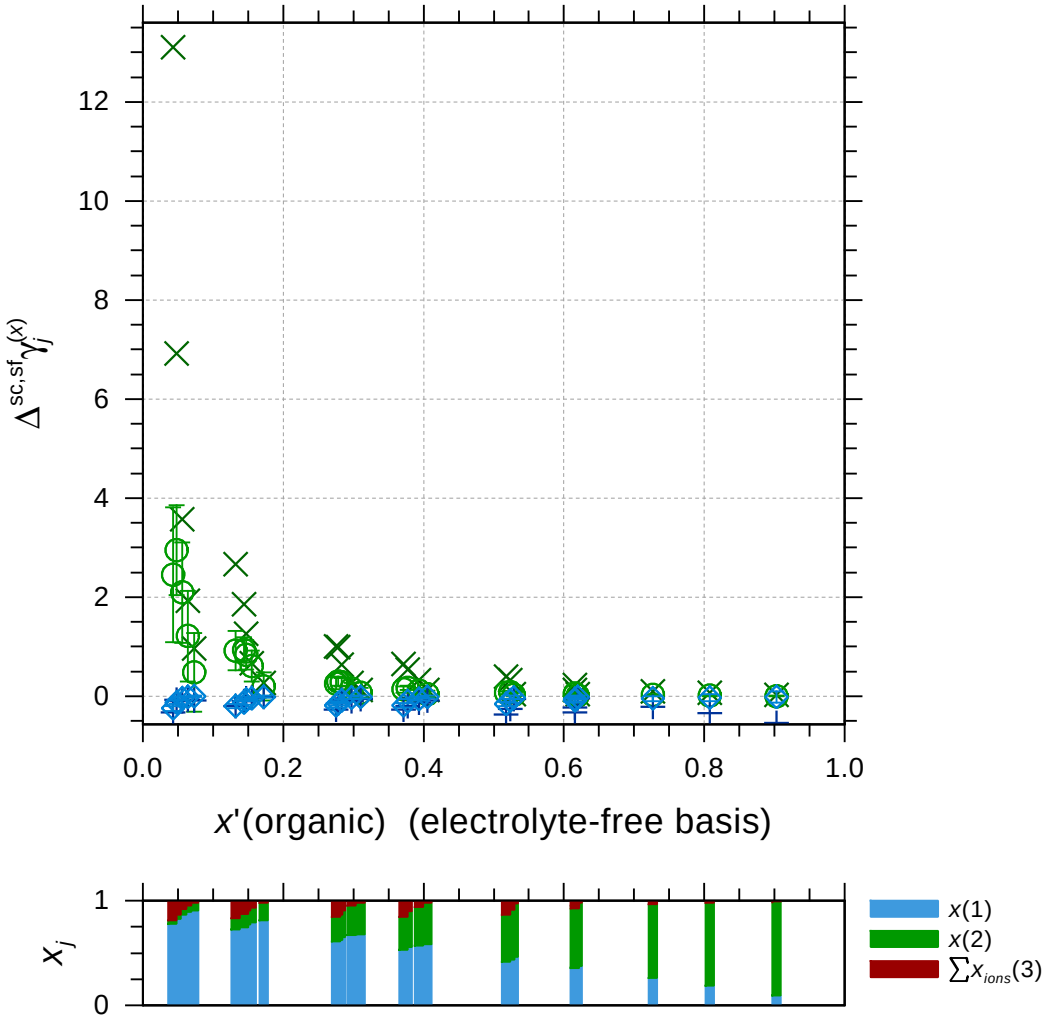


initial weighting of dataset:
$w^{init}(0100)$ = 0.500
dataset contribution to F_{obj}:
fval(0100) = 5.0767E-01
rel. contribution = 0.2414 %

Fig. S0075 (AIOMFAC_output_0101)

H_2O (1) + 2-Propanol (2) + LiBr (3)

Temperature range: 354 -- 357 K

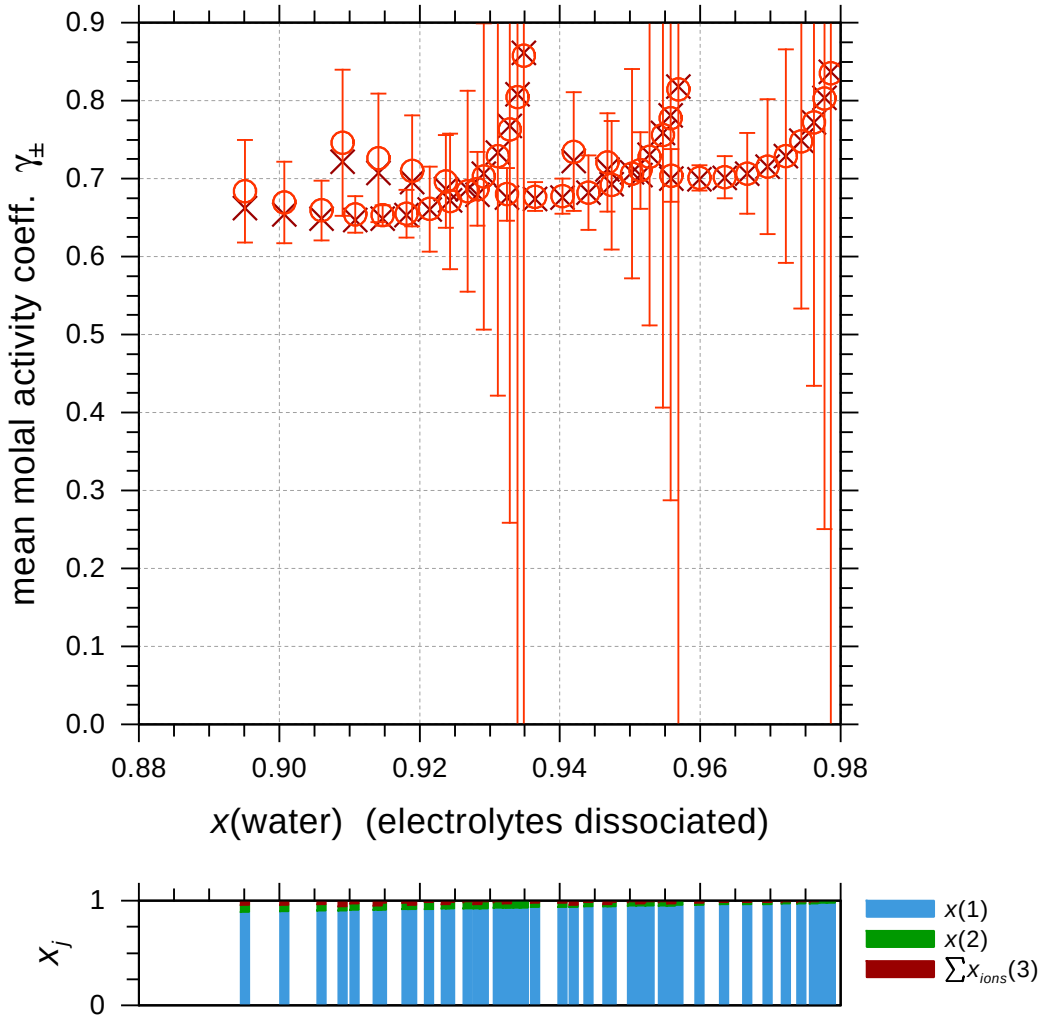


initial weighting of dataset:
$w^{init}(0101)$ = 0.500
dataset contribution to F_{obj}:
fval(0101) = 3.5522E-01
rel. contribution = 0.1689 %

Fig. S0076 (AIOMFAC_output_1027)

H_2O (1) + Ethanol (2) + LiCl (3)

Temperature: 298 K

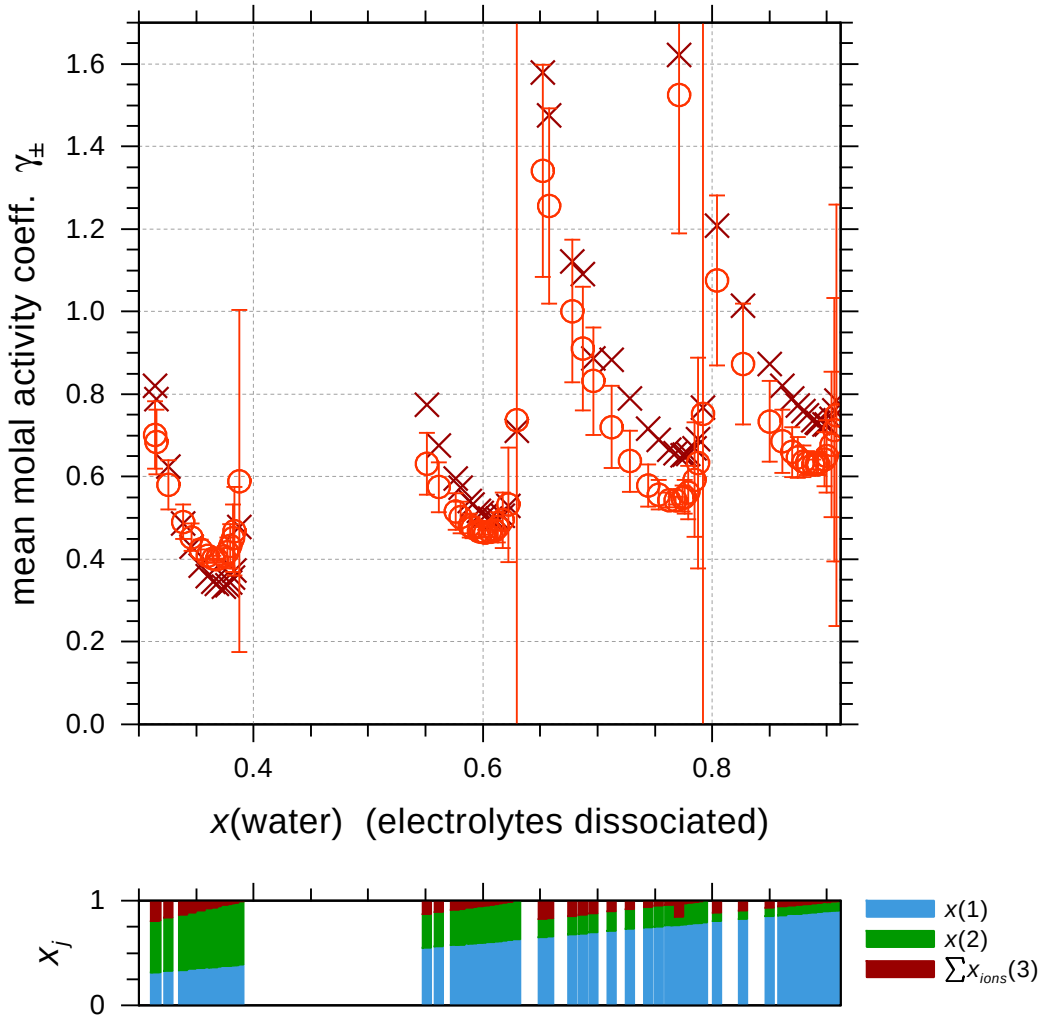


initial weighting of dataset:
$w^{init}(1027)$ = 2.000
dataset contribution to F_{obj}:
fval(1027) = 2.1274E-03
rel. contribution = 0.0010 %

Fig. S0077 (AIOMFAC_output_1028)

H_2O (1) + Ethanol (2) + LiCl (3)

Temperature: 298 K

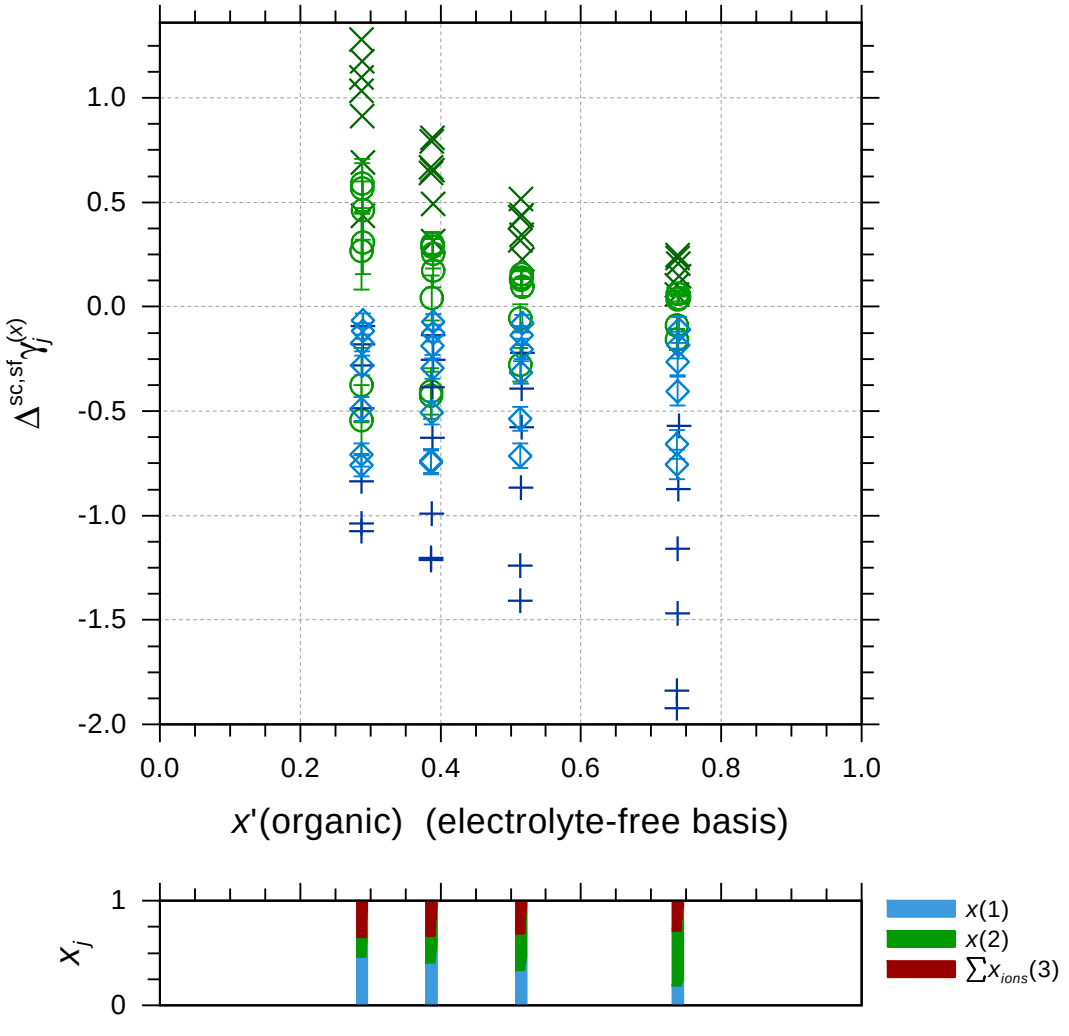


initial weighting of dataset:
$w^{init}(1028)$ = 2.000
dataset contribution to F_{obj}:
fval(1028) = 3.3211E-01
rel. contribution = 0.1579 %

Fig. S0078 (AIOMFAC_output_0061)

H_2O (1) + 2-Propanol (2) + LiCl (3)

Temperature: 348 K

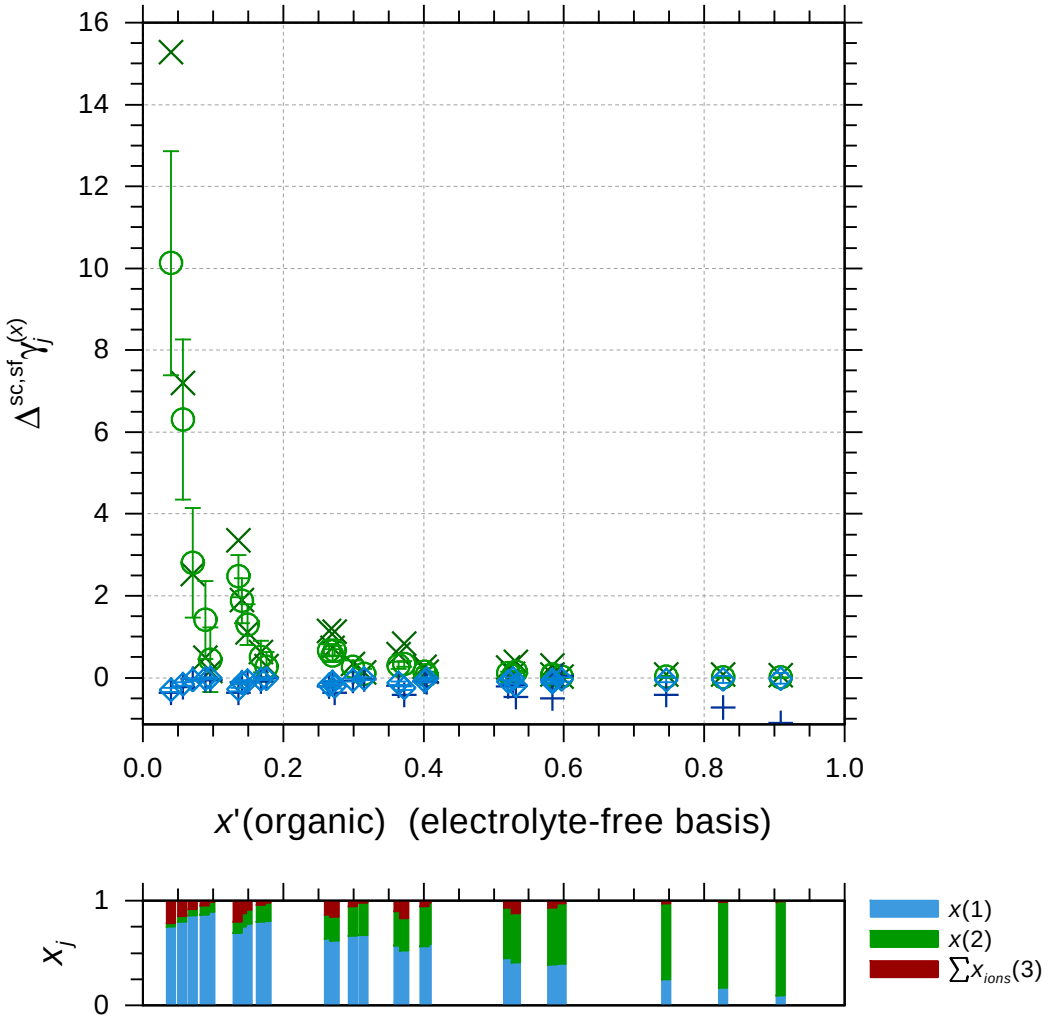


initial weighting of dataset:
$w^{init}(0061)$ = 0.500
dataset contribution to F_{obj}:
fval(0061) = 8.3569E-01
rel. contribution = 0.3974 %

Fig. S0079 (AIOMFAC_output_0062)

H_2O (1) + 2-Propanol (2) + LiCl (3)

Temperature range: 354 -- 358 K



initial weighting of dataset:

w^{init}(0062) = 0.500

dataset contribution to F_{obj}:

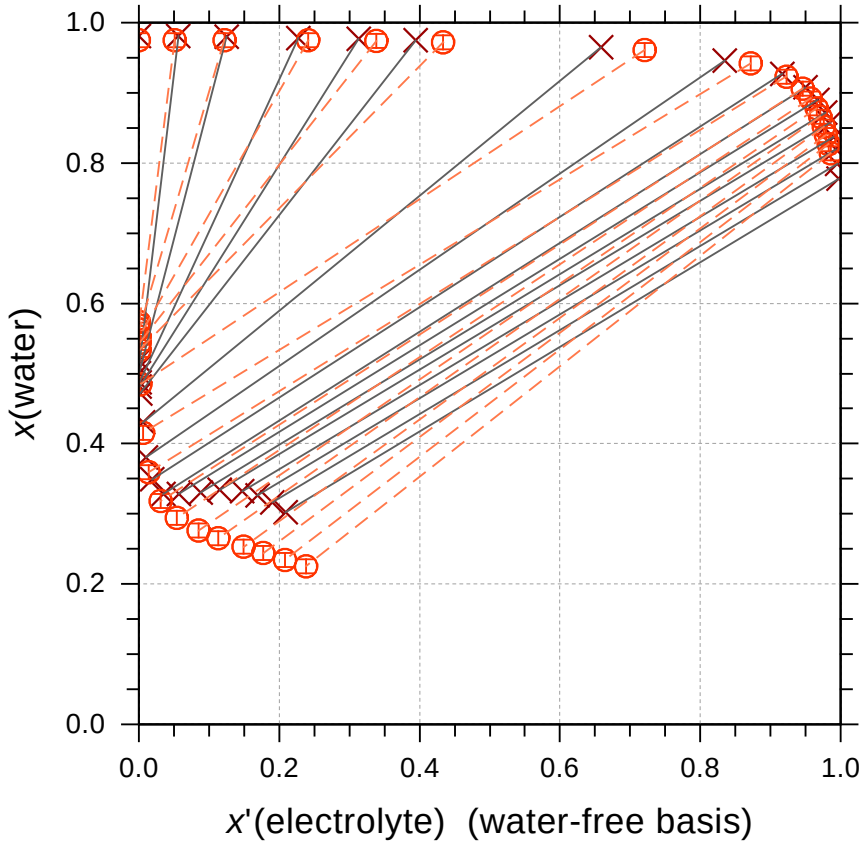
fval(0062) = 2.1522E-01

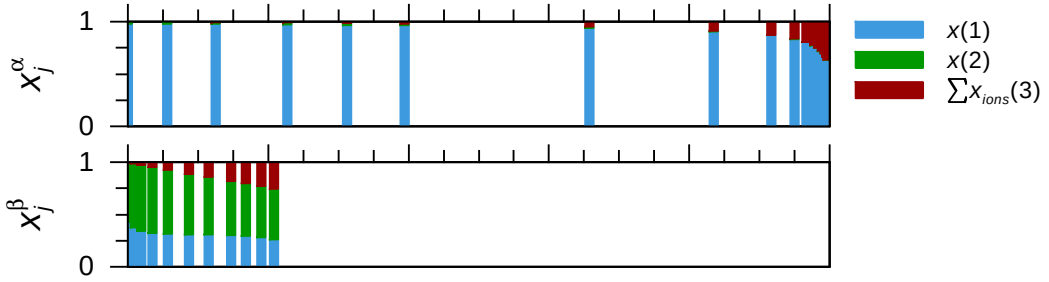
rel. contribution = 0.1023 %

Fig. S0080 (AIOMFAC_output_0972)

H_2O (1) + 1-Butanol (2) + LiCl (3)

Temperature: 298 K





left y-axis:

× LiCl+1-Butanol+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0972) = 0.100

dataset contribution to F_{obj}:

fval(0972) = 1.1566E-01

rel. contribution = 0.0550 %

Fig. S0080a (AIOMFAC_output_0972)

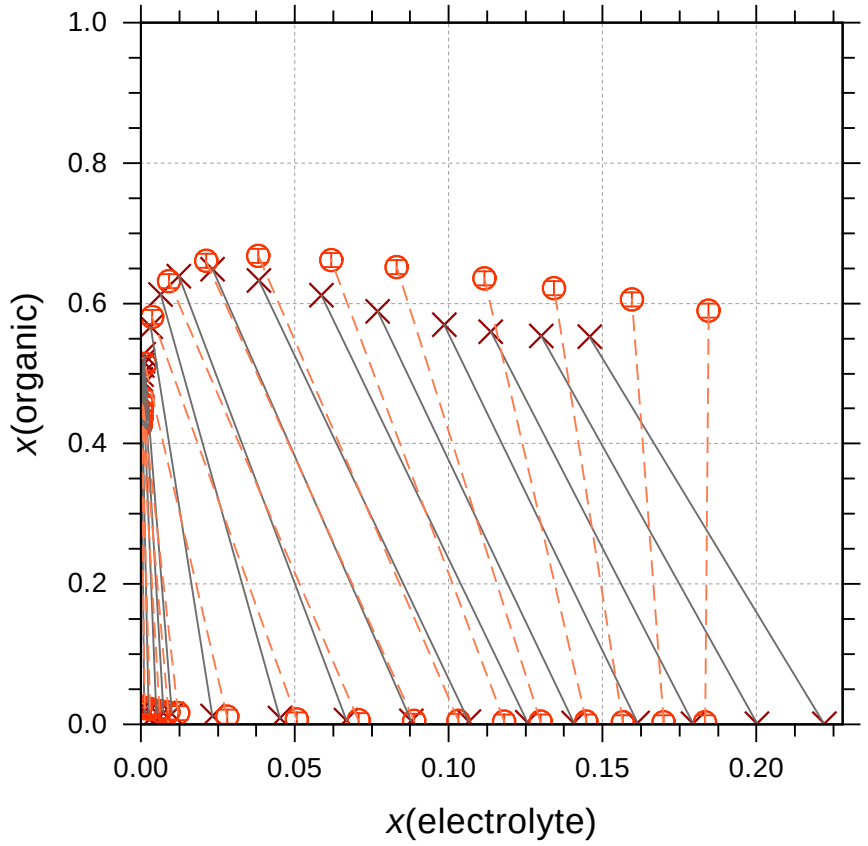
H_2O (1) + 1-Butanol (2) + LiCl (3)

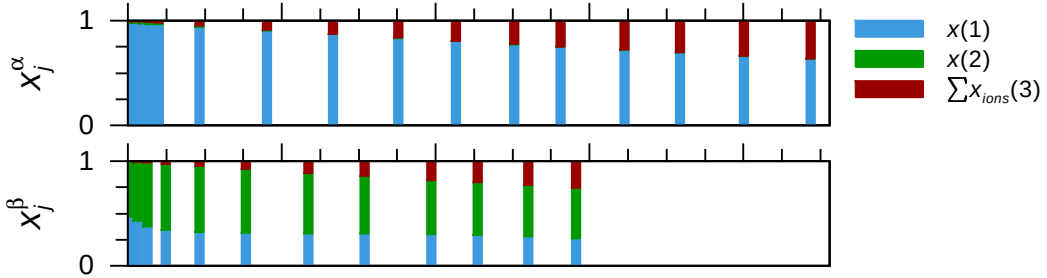
Temperature: 298 K

left y-axis:

× LiCl+1-Butanol+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0972) = 0.100

dataset contribution to F_{obj}:

fval(0972) = 1.1566E-01

rel. contribution = 0.0550 %

Fig. S0081 (AIOMFAC_output_0973)

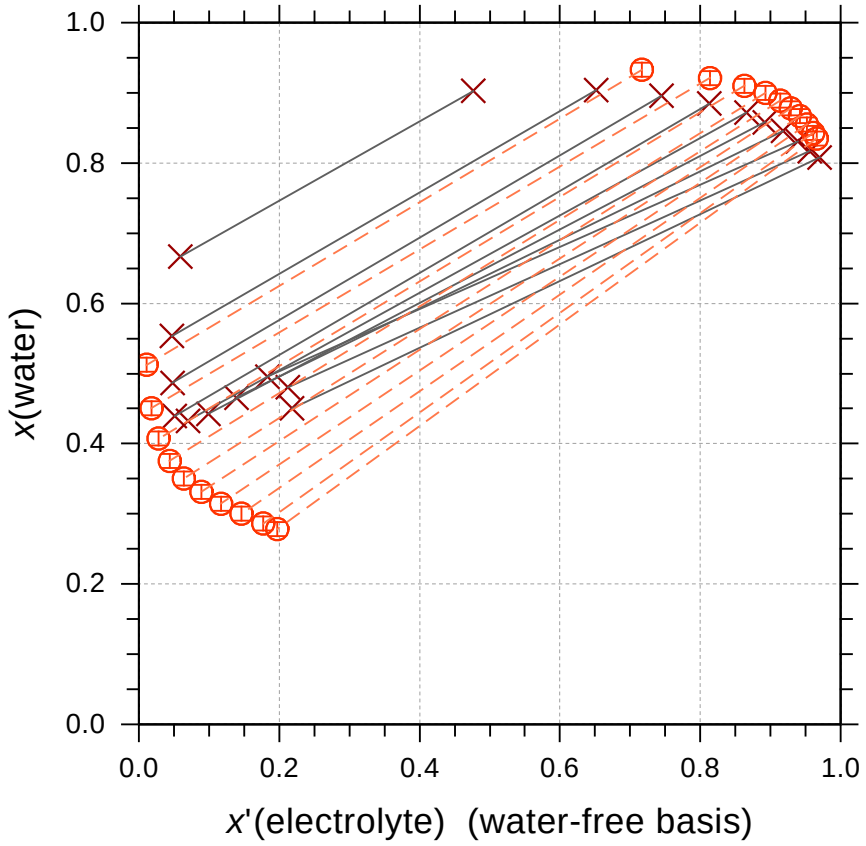
H_2O (1) + *tert*-Butanol (2) + LiCl (3)

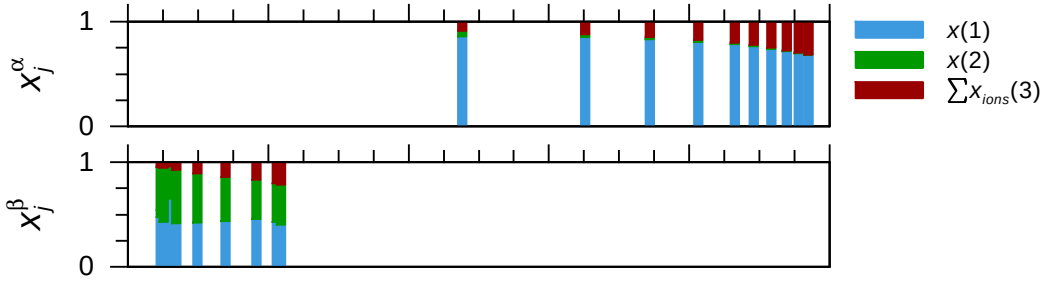
Temperature: 298 K

left y-axis:

× LiCl+tert-Butanol+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0973)$ = 0.100

dataset contribution to F_{obj}:

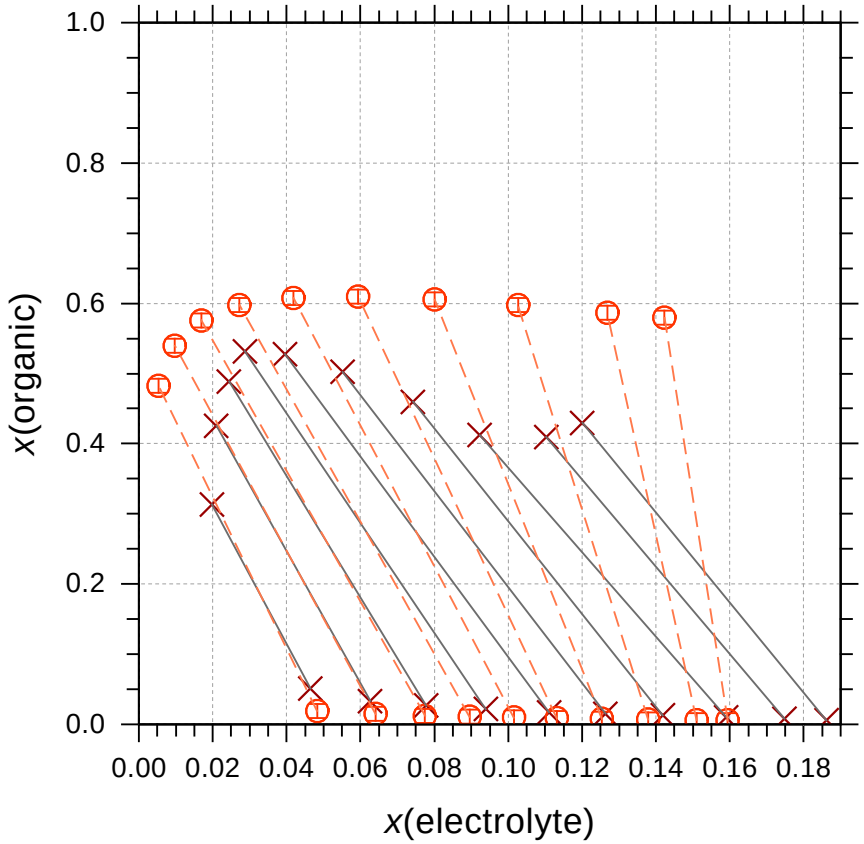
fval(0973) = 3.7753E-01

rel. contribution = 0.1795 %

Fig. S0081a (AIOMFAC_output_0973)

H_2O (1) + *tert*-Butanol (2) + LiCl (3)

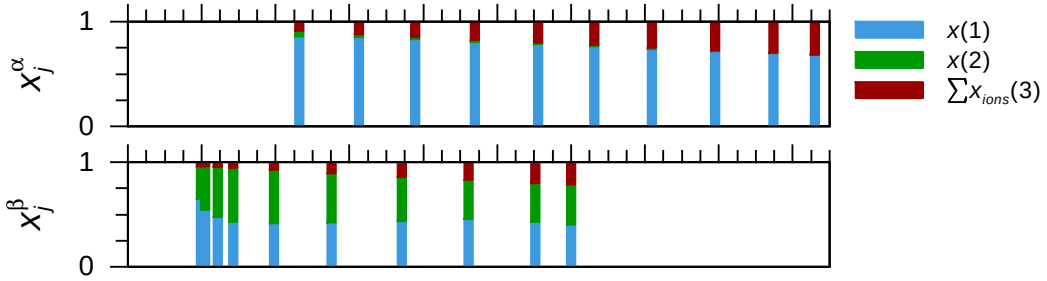
Temperature: 298 K



left y-axis:

× LiCl+tert-Butanol+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition

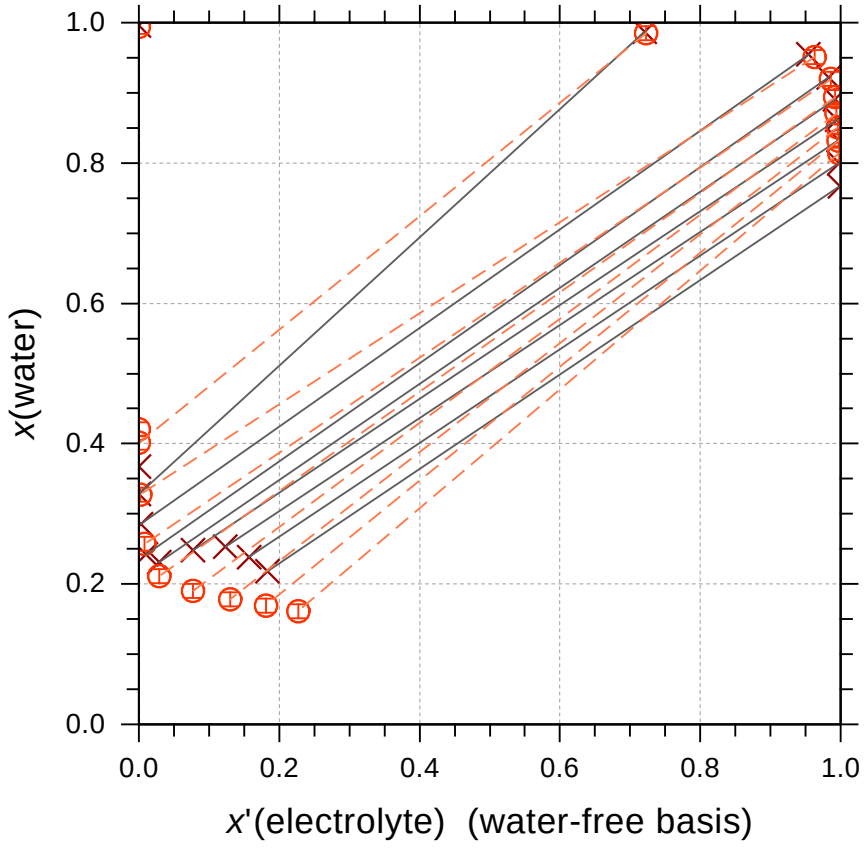


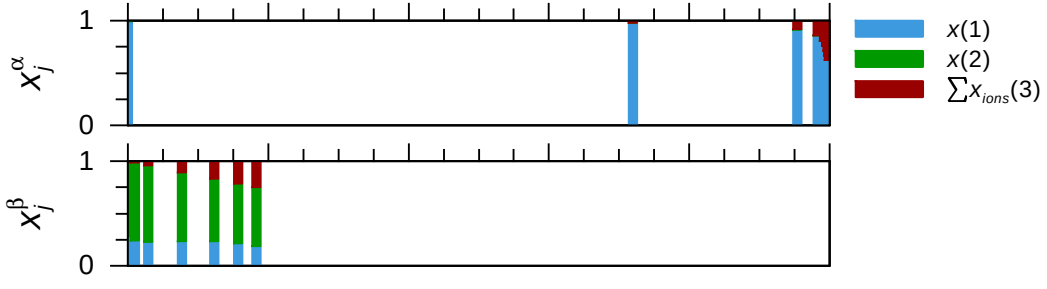
initial weighting of dataset:
w^{init}(0973) = 0.100
dataset contribution to F_{obj}:
fval(0973) = 3.7753E-01
rel. contribution = 0.1795 %

Fig. S0082 (AIOMFAC_output_0994)

H_2O (1) + 1-Pentanol (2) + LiCl (3)

Temperature: 298 K





left y-axis:

× LiCl+1-Pentanol+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0994) = 0.100

dataset contribution to F_{obj}:

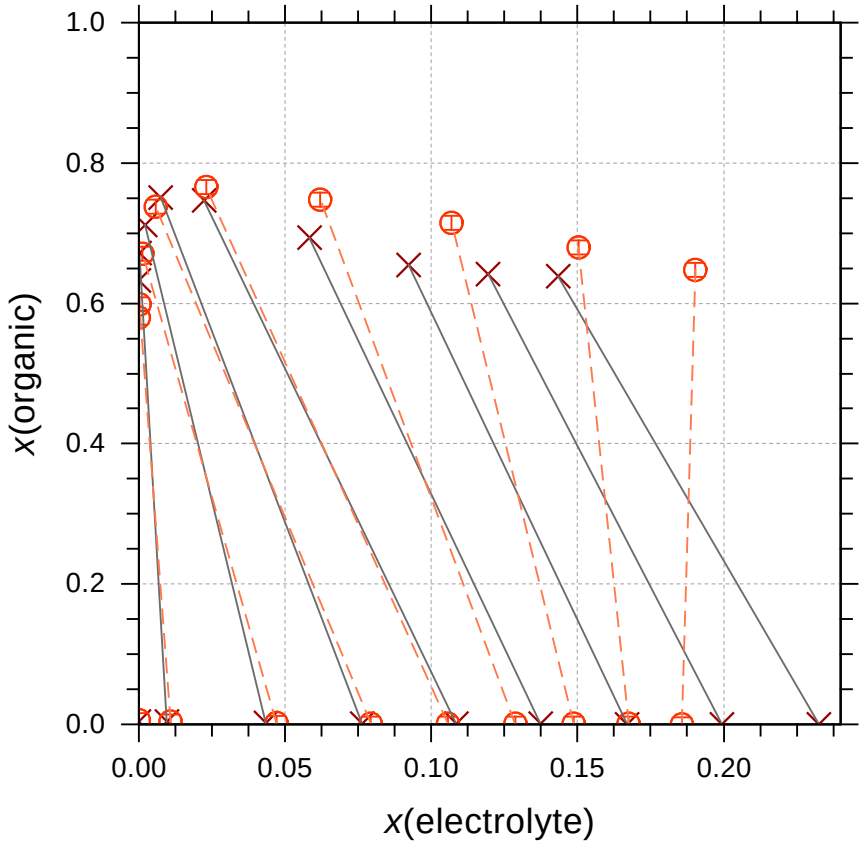
fval(0994) = 4.9485E-01

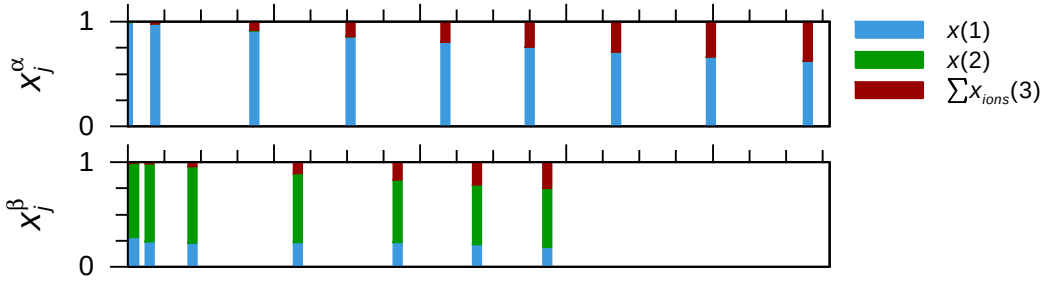
rel. contribution = 0.2353 %

Fig. S0082a (AIOMFAC_output_0994)

H_2O (1) + 1-Pentanol (2) + LiCl (3)

Temperature: 298 K





initial weighting of dataset:
w^{init}(0994) = 0.100
dataset contribution to F_{obj}:
fval(0994) = 4.9485E-01
rel. contribution = 0.2353 %

Fig. S0083 (AIOMFAC_output_0995)

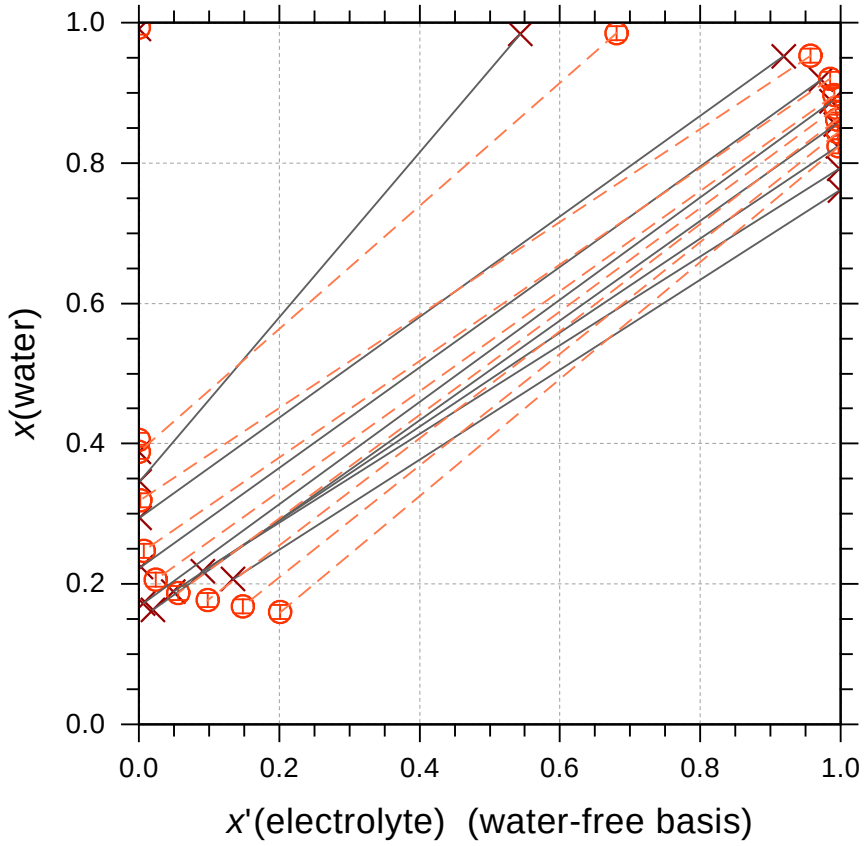
H_2O (1) + 2-Pentanol (2) + LiCl (3)

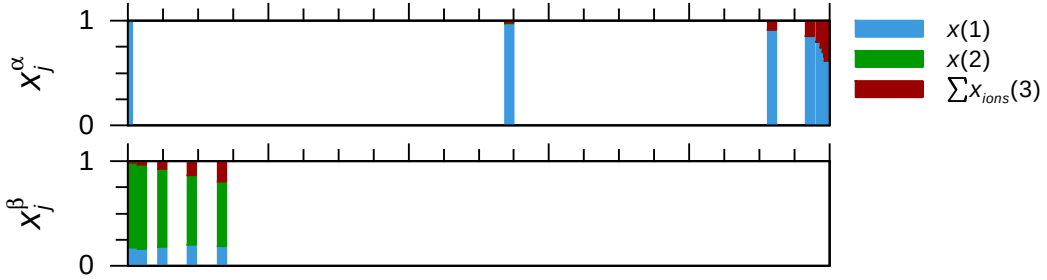
Temperature: 298 K

left y-axis:

× LiCl+2-Pentanol+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0995) = 0.100

dataset contribution to F_{obj}:

fval(0995) = 9.1977E-01

rel. contribution = 0.4374 %

Fig. S0083a (AIOMFAC_output_0995)

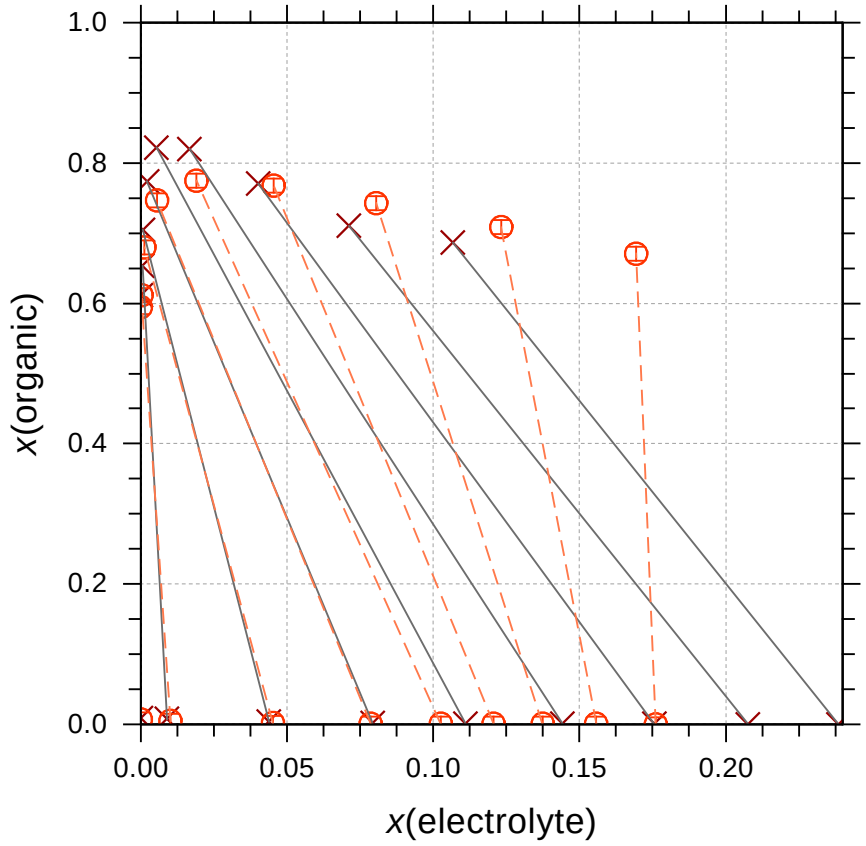
H_2O (1) + 2-Pentanol (2) + LiCl (3)

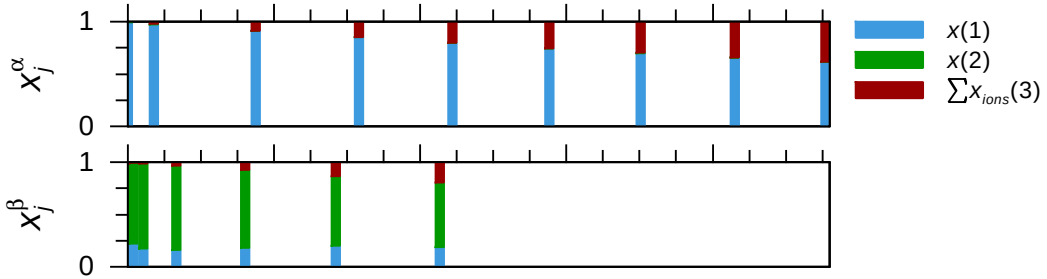
Temperature: 298 K

left y-axis:

× LiCl+2-Pentanol+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0995) = 0.100

dataset contribution to F_{obj}:

fval(0995) = 9.1977E-01

rel. contribution = 0.4374 %

Fig. S0084 (AIOMFAC_output_0996)

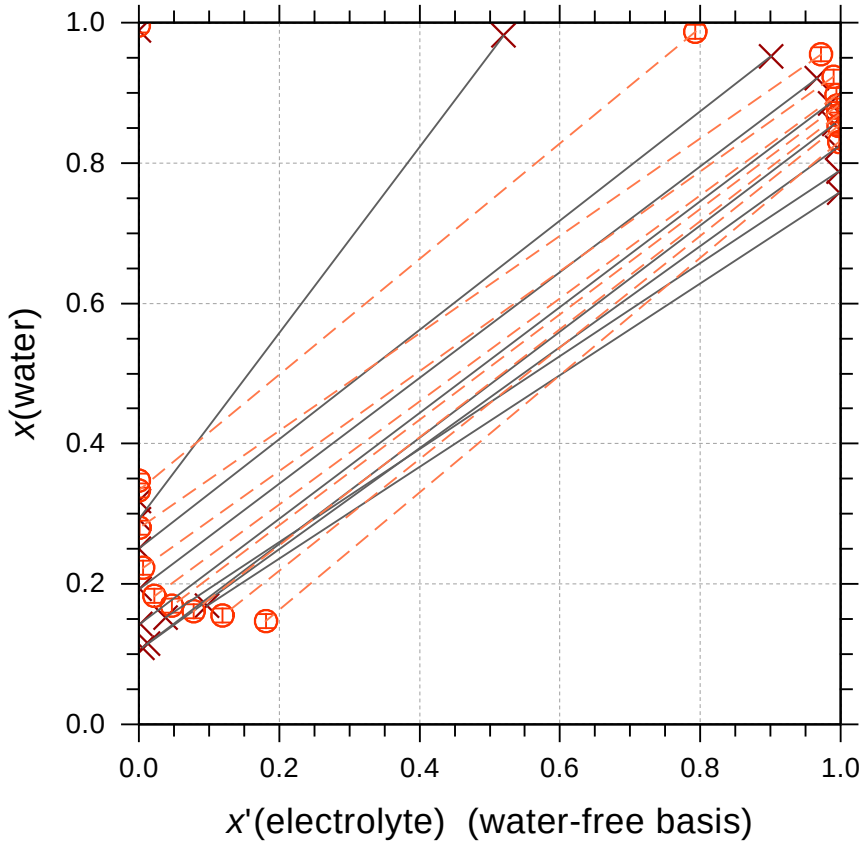
H_2O (1) + 3-Pentanol (2) + LiCl (3)

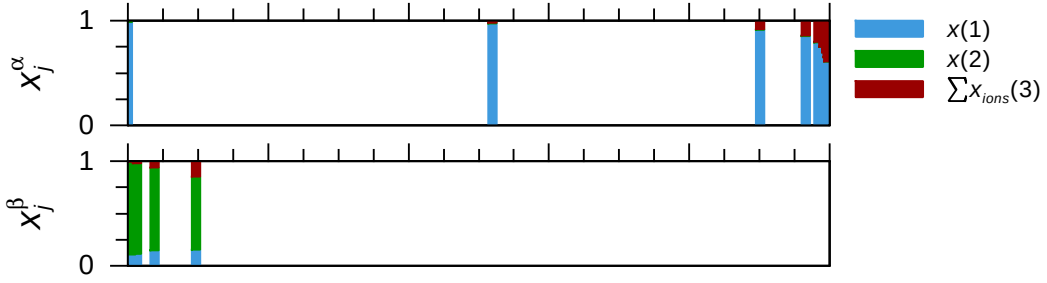
Temperature: 298 K

left y-axis:

× LiCl+3-Pentanol+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0996)$ = 0.100

dataset contribution to F_{obj}:

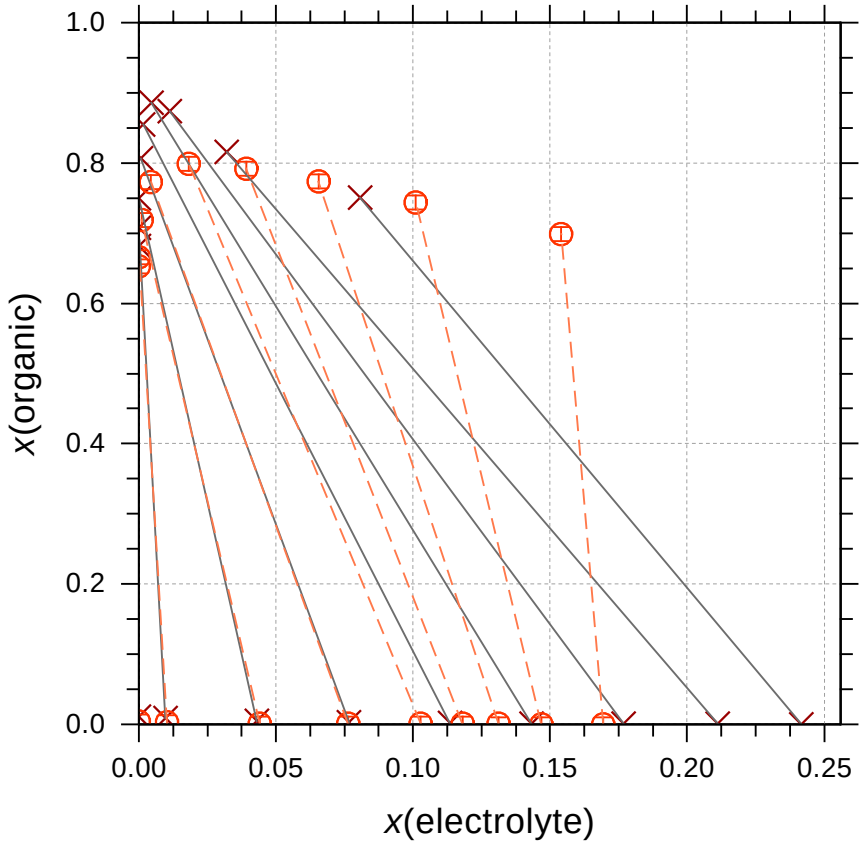
fval(0996) = 1.0528E+00

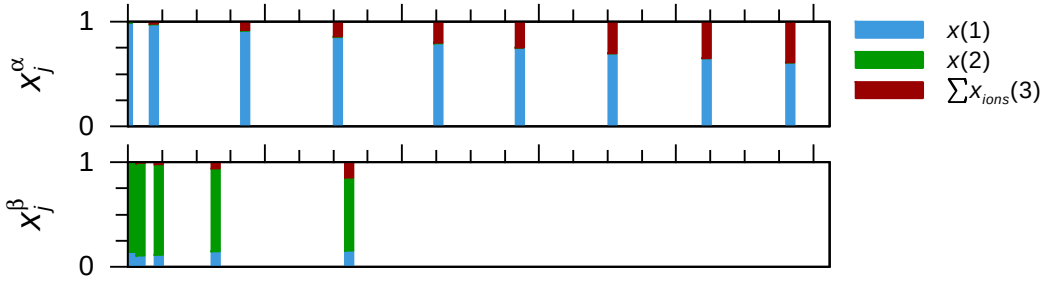
rel. contribution = 0.5006 %

Fig. S0084a (AIOMFAC_output_0996)

H_2O (1) + 3-Pentanol (2) + LiCl (3)

Temperature: 298 K



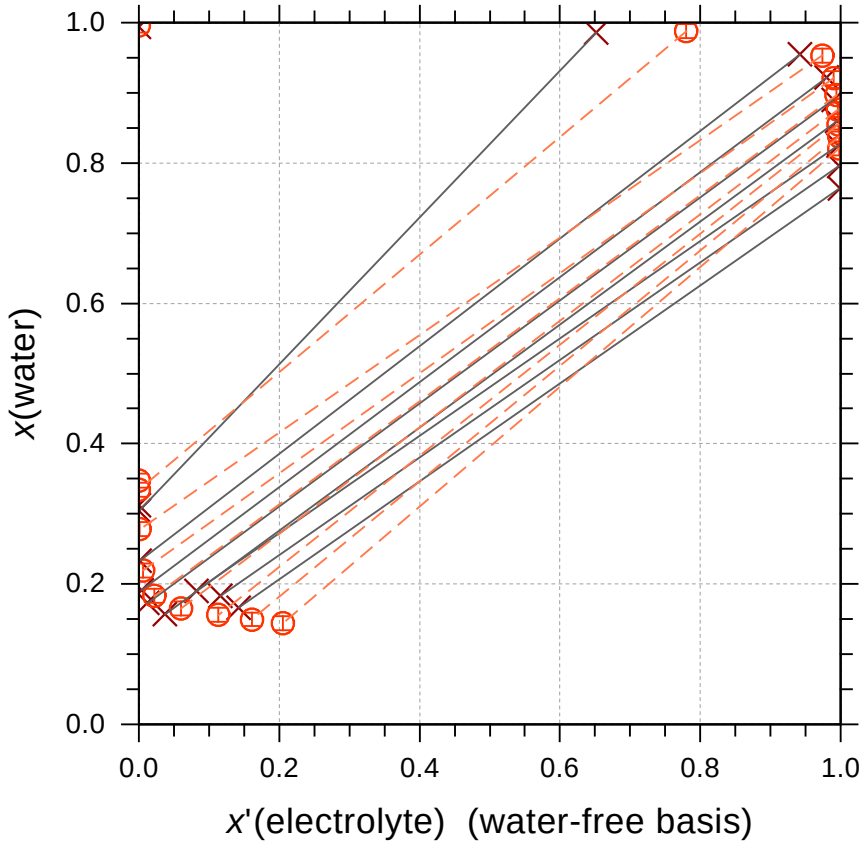


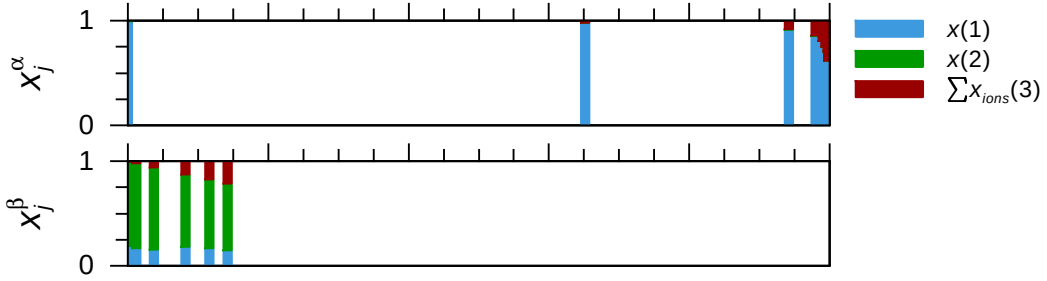
initial weighting of dataset:
w^{init}(0996) = 0.100
dataset contribution to F_{obj}:
fval(0996) = 1.0528E+00
rel. contribution = 0.5006 %

Fig. S0085 (AIOMFAC_output_0997)

H_2O (1) + 2-Methyl-1-butanol (2) + LiCl (3)

Temperature: 298 K





left y-axis:

× LiCl+2-Methyl-1-butanol+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0997)$ = 0.100

dataset contribution to F_{obj}:

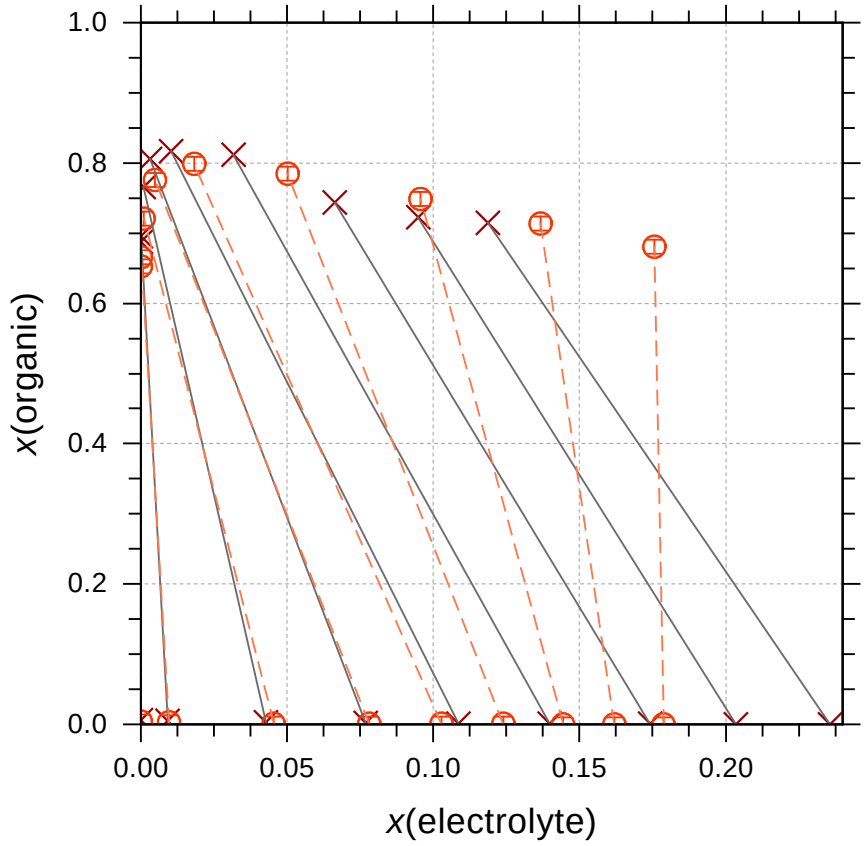
fval(0997) = 6.6557E-01

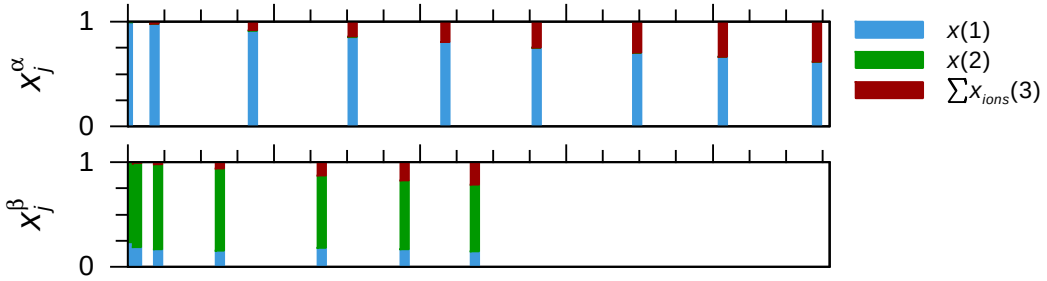
rel. contribution = 0.3165 %

Fig. S0085a (AIOMFAC_output_0997)

H_2O (1) + 2-Methyl-1-butanol (2) + LiCl (3)

Temperature: 298 K



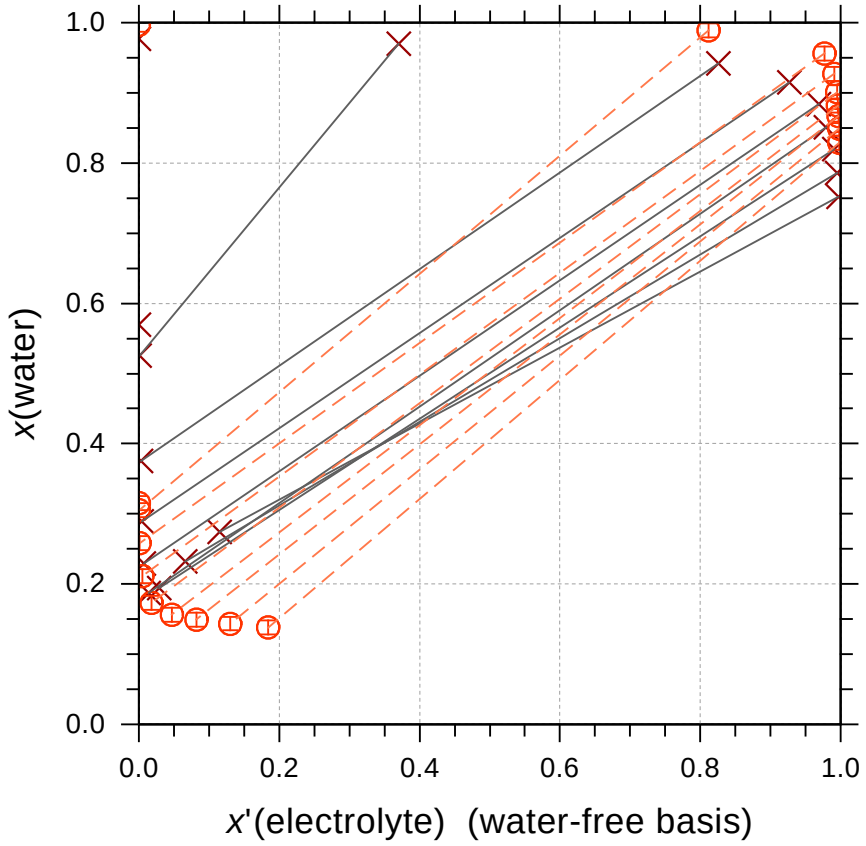


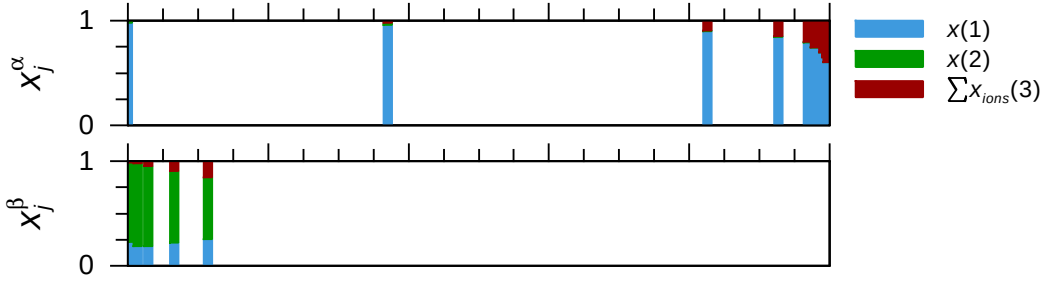
initial weighting of dataset:
w^{init}(0997) = 0.100
dataset contribution to F_{obj}:
fval(0997) = 6.6557E-01
rel. contribution = 0.3165 %

Fig. S0086 (AIOMFAC_output_0998)

H_2O (1) + 2-Methyl-2-butanol (2) + LiCl (3)

Temperature: 298 K





left y-axis:

× LiCl+2-Methyl-2-butanol+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:
w^{init}(0998) = 0.100
dataset contribution to F_{obj}:
fval(0998) = 2.1018E+00
rel. contribution = 0.9995 %

Fig. S0086a (AIOMFAC_output_0998)

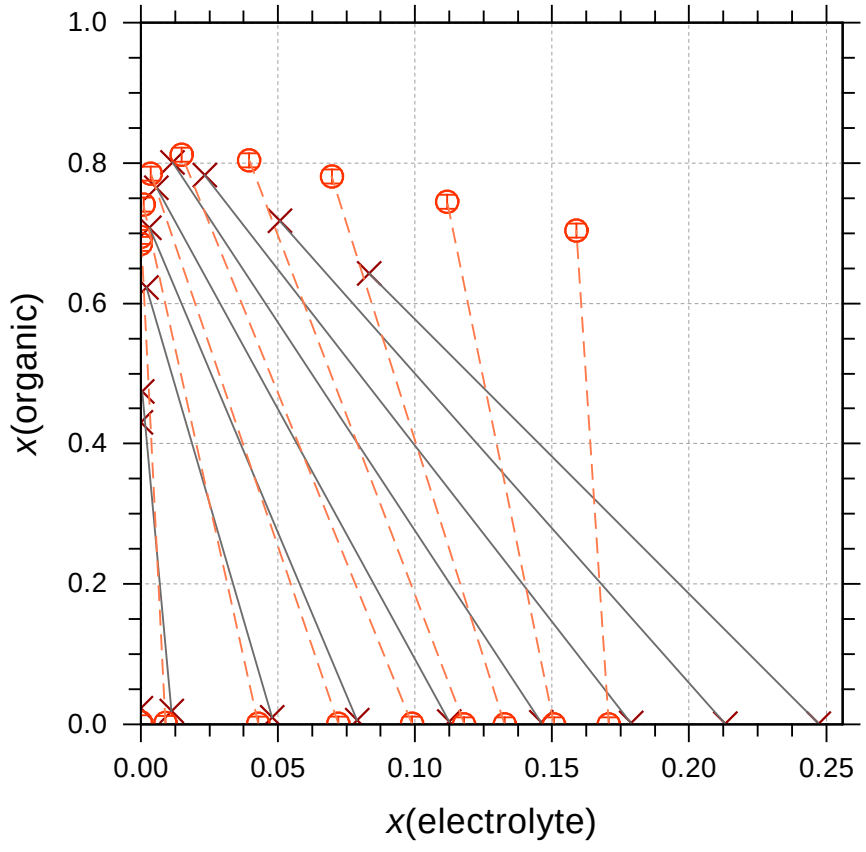
H_2O (1) + 2-Methyl-2-butanol (2) + LiCl (3)

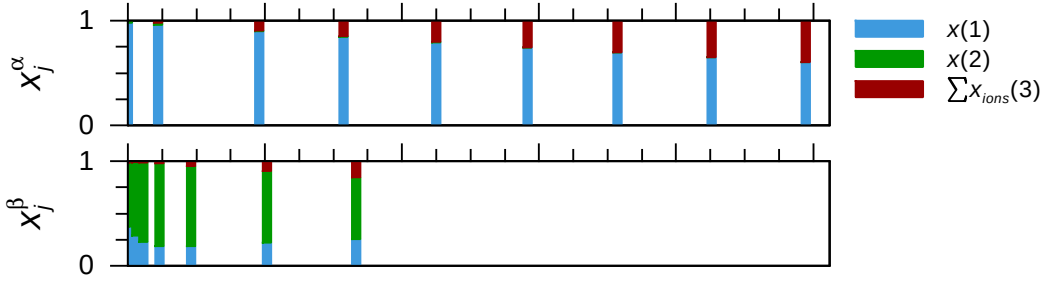
Temperature: 298 K

left y-axis:

× LiCl+2-Methyl-2-butanol+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0998)$ = 0.100

dataset contribution to F_{obj}:

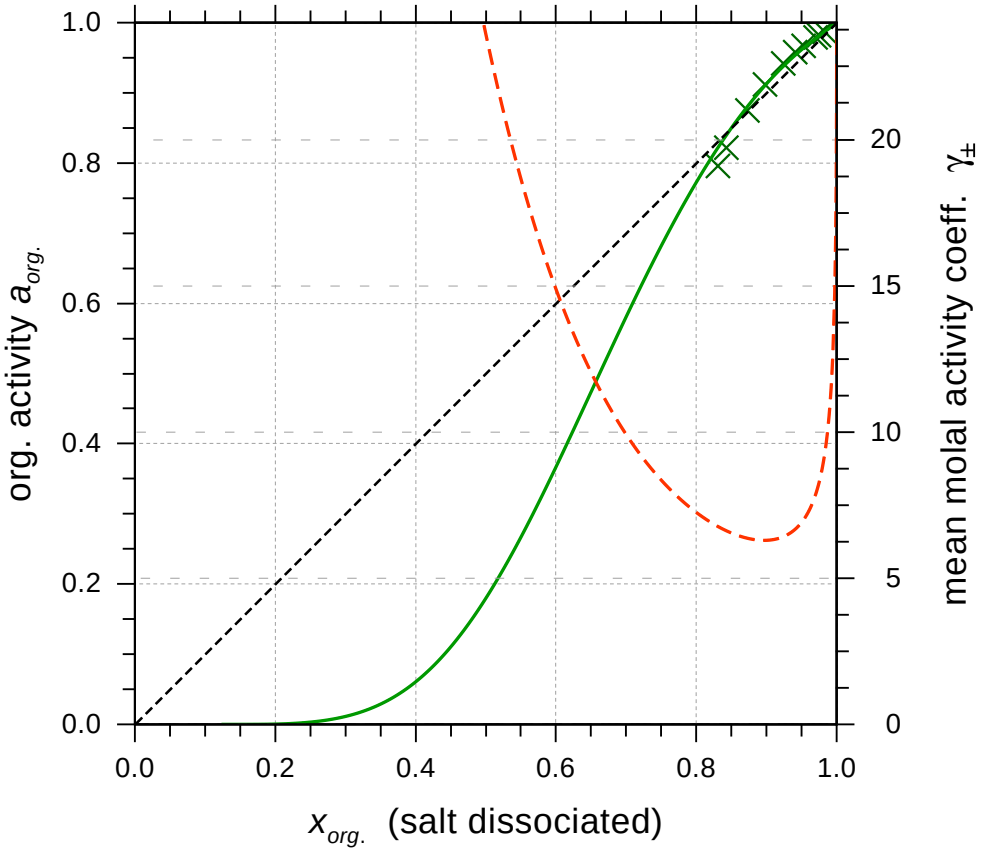
fval(0998) = 2.1018E+00

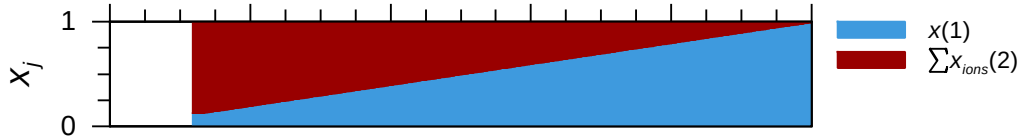
rel. contribution = 0.9995 %

Fig. S0087 (AIOMFAC_output_0936)

Ethanol (1) + $LiNO_3$ (2)

Temperature: 298 K





left y-axis:

× LiNO3+Ethanol_activity_Verevkin

AIOMFAC org. activity $a_{org.}$

ideal $a_{org.}$

right y-axis:

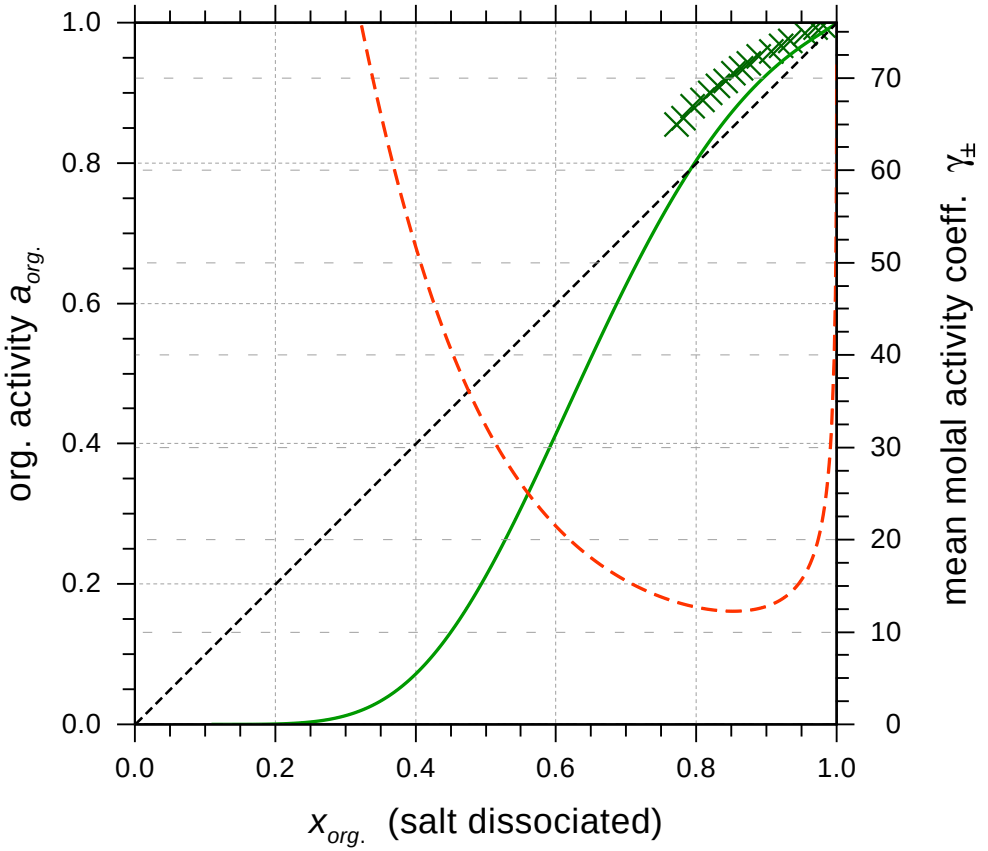
AIOMFAC mean molal activity coeff. $\gamma_{\pm}$

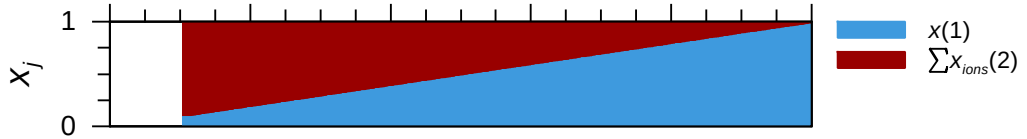
initial weighting of dataset:
$w^{init}(0936)$ = 0.500
dataset contribution to F_{obj}:
fval(0936) = 7.5085E-04
rel. contribution = 0.0004 %

Fig. S0088 (AIOMFAC_output_0937)

1-Propanol (1) + $LiNO_3$ (2)

Temperature: 298 K





left y-axis:

× LiNO3+1-Propanol_activity_Vercher

AIOMFAC org. activity $a_{org.}$

ideal $a_{org.}$

right y-axis:

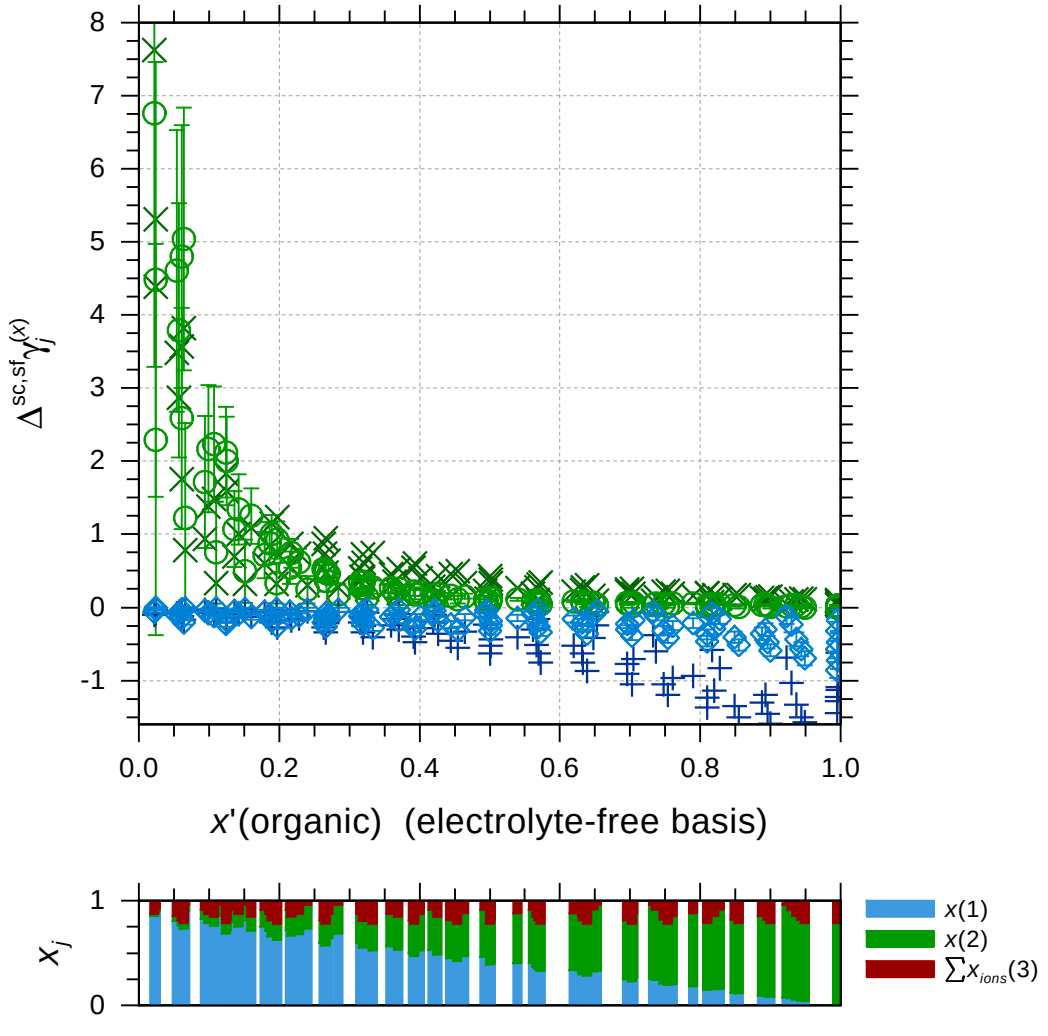
AIOMFAC mean molal activity coeff. $\gamma_{\pm}$

initial weighting of dataset:
w^{init}(0937) = 0.500
dataset contribution to F_{obj}:
fval(0937) = 1.8096E-02
rel. contribution = 0.0086 %

Fig. S0089 (AIOMFAC_output_0939)

H_2O (1) + 1-Propanol (2) + $LiNO_3$ (3)

Temperature range: 361 -- 374 K



initial weighting of dataset:

w^{init}(0939) = 0.500

dataset contribution to F_{obj}:

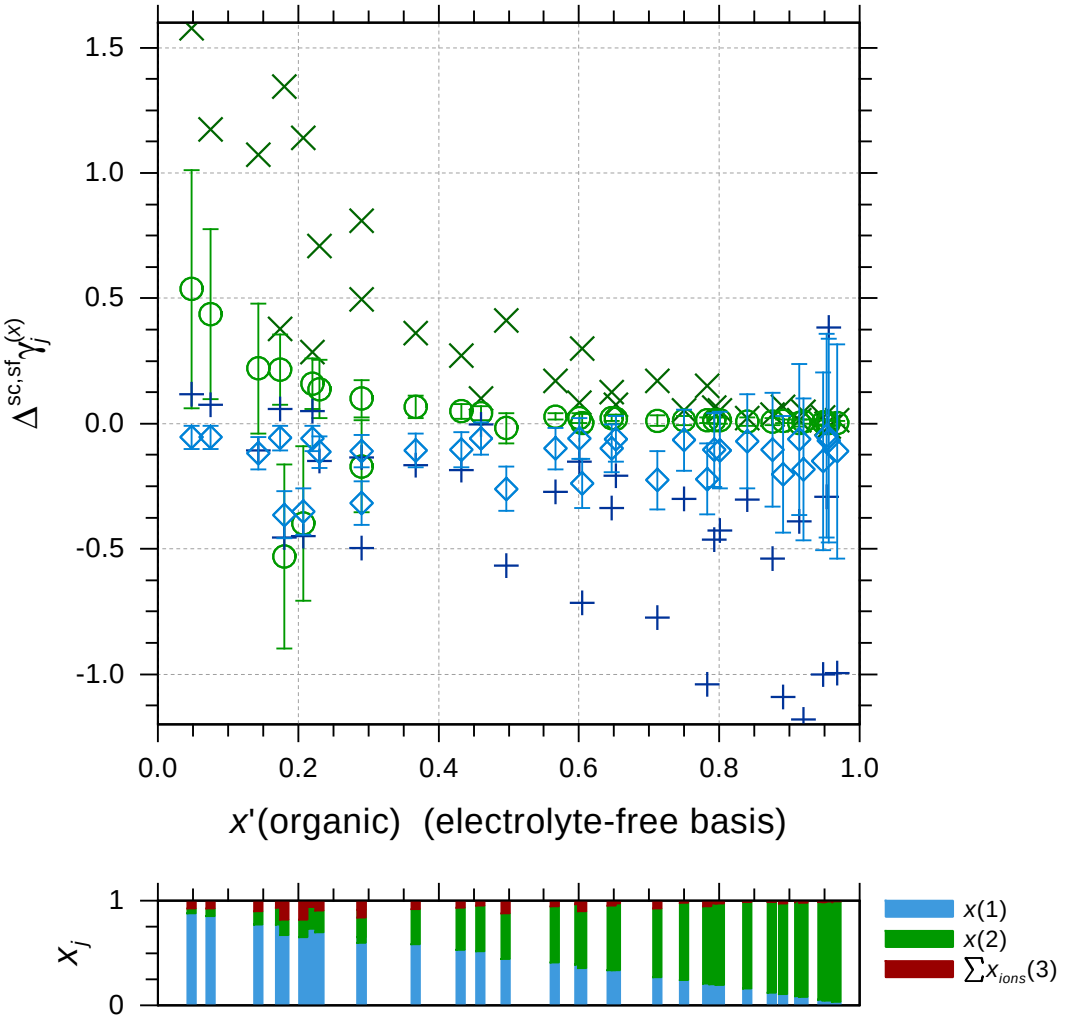
fval(0939) = 3.1027E-01

rel. contribution = 0.1475 %

Fig. S0090 (AIOMFAC_output_0408)

H_2O (1) + 2-Propanol (2) + $MgBr_2$ (3)

Temperature range: 354 -- 359 K



initial weighting of dataset:
$w^{init}(0408)$ = 0.500
dataset contribution to F_{obj}:
fval(0408) = 4.9771E-01
rel. contribution = 0.2367 %

Fig. S0091 (AIOMFAC_output_0363)

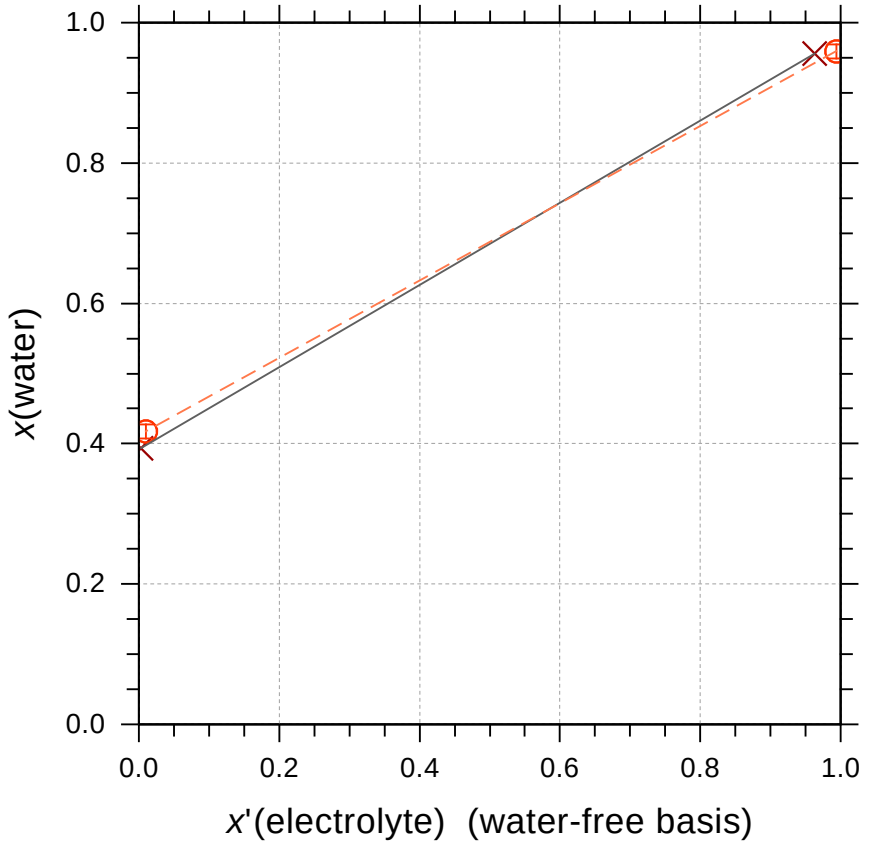
H_2O (1) + 1,3-Nonanediol (2) + $MgCl_2$ (3)

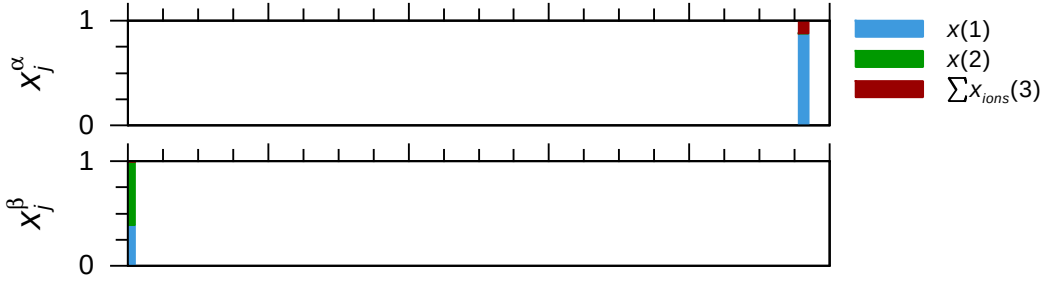
Temperature: 298 K

left y-axis:

× MgCl2+1,3-Nonanediol+Water_LLE_Putnin

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0363) = 1.000

dataset contribution to F_{obj}:

fval(0363) = 6.9904E-02

rel. contribution = 0.0332 %

Fig. S0091a (AIOMFAC_output_0363)

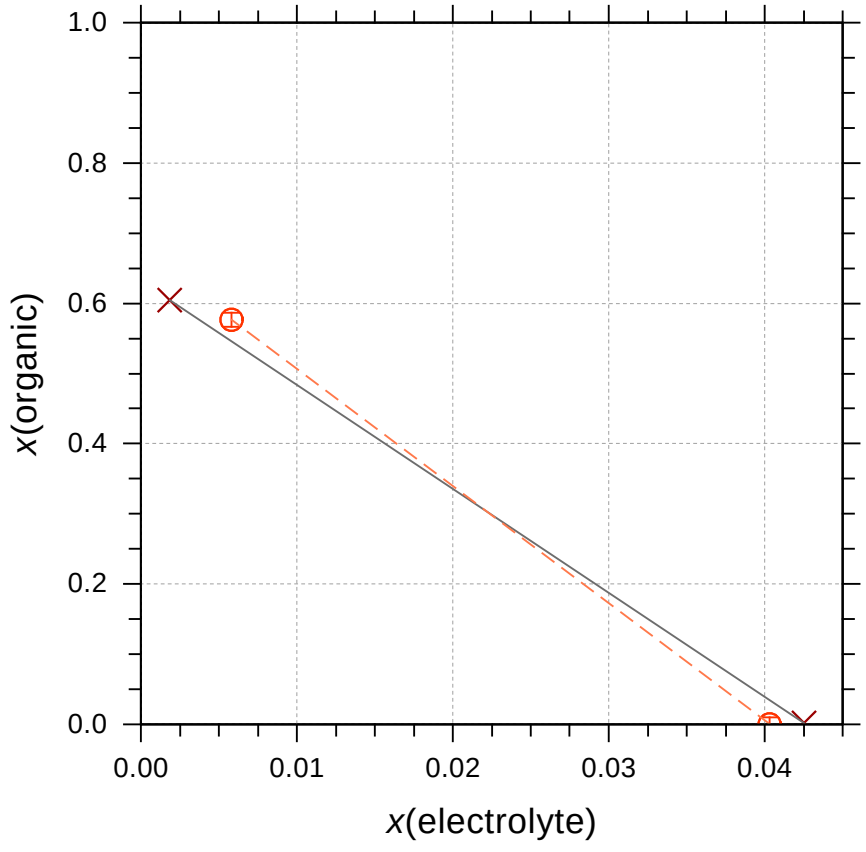
H_2O (1) + 1,3-Nonanediol (2) + $MgCl_2$ (3)

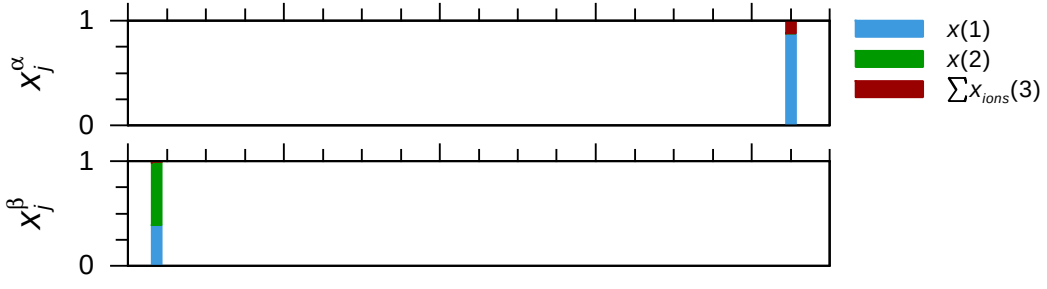
Temperature: 298 K

left y-axis:

× MgCl2+1,3-Nonanediol+Water_LLE_Putnin

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0363) = 1.000

dataset contribution to F_{obj}:

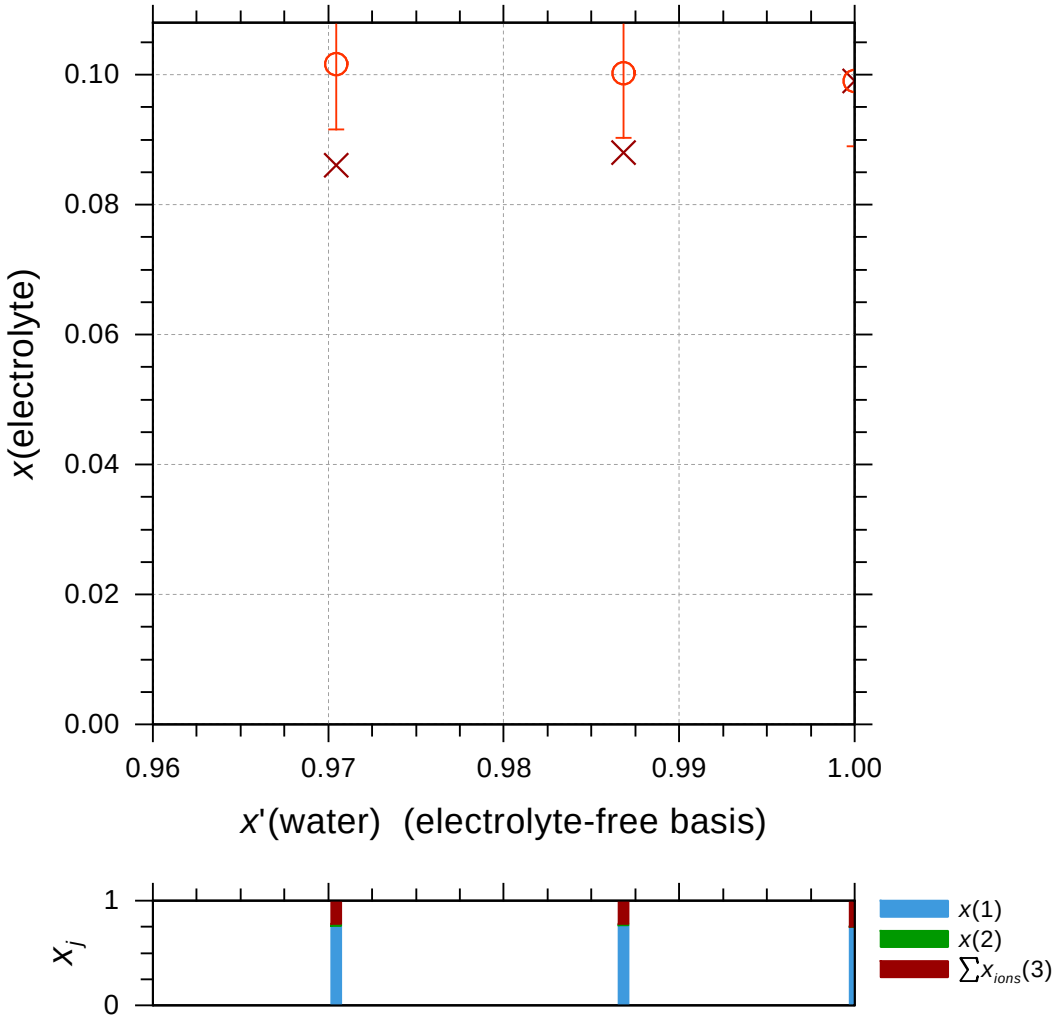
fval(0363) = 6.9904E-02

rel. contribution = 0.0332 %

Fig. S0092 (AIOMFAC_output_0369)

H_2O (1) + 2-Propanol (2) + $MgCl_2$ (3)

Temperature: 313 K

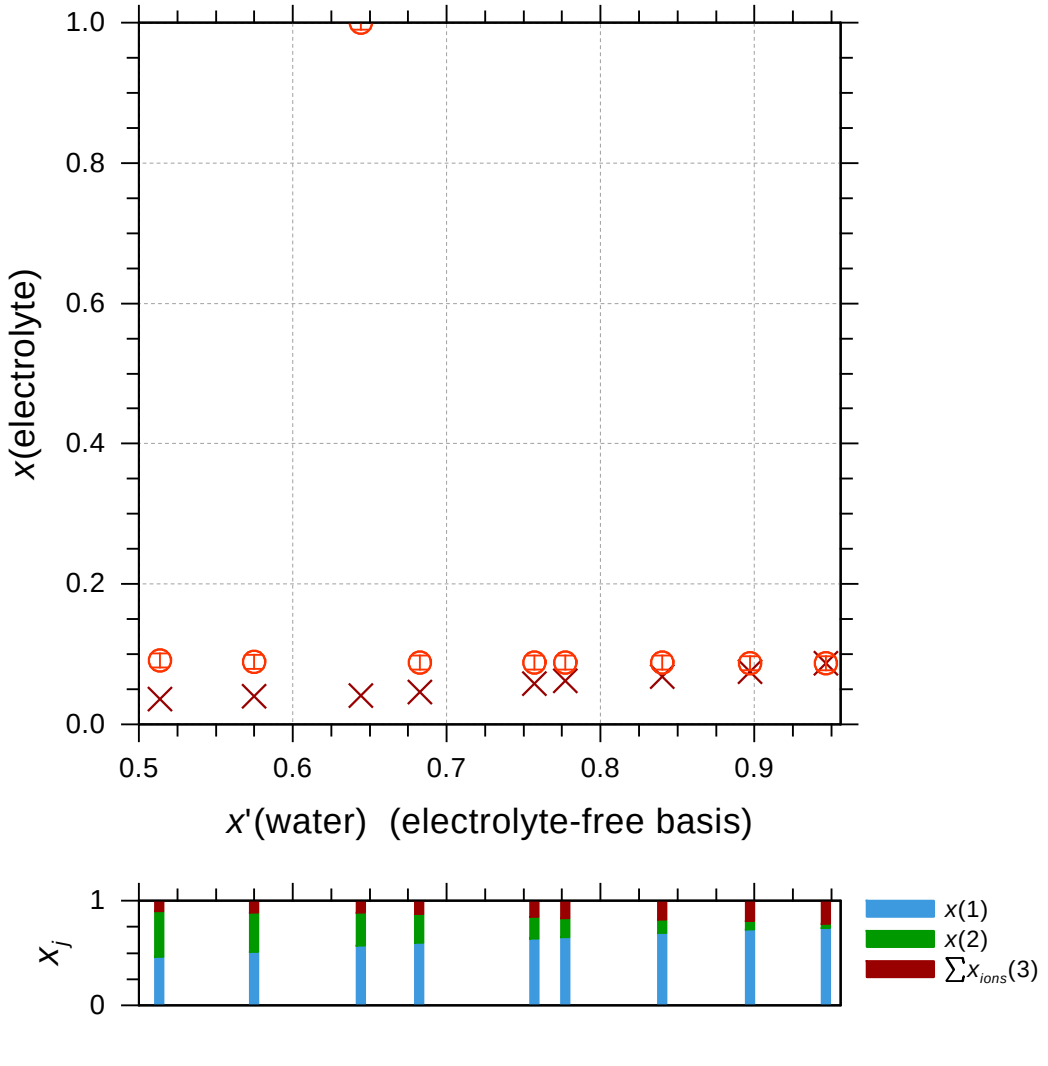


initial weighting of dataset:
w^{init}(0369) = 0.500
dataset contribution to F_{obj}:
fval(0369) = 2.1213E-02
rel. contribution = 0.0101 %

Fig. S0093 (AIOMFAC_output_0370)

H_2O (1) + 2-Propanol (2) + $MgCl_2$ (3)

Temperature: 313 K

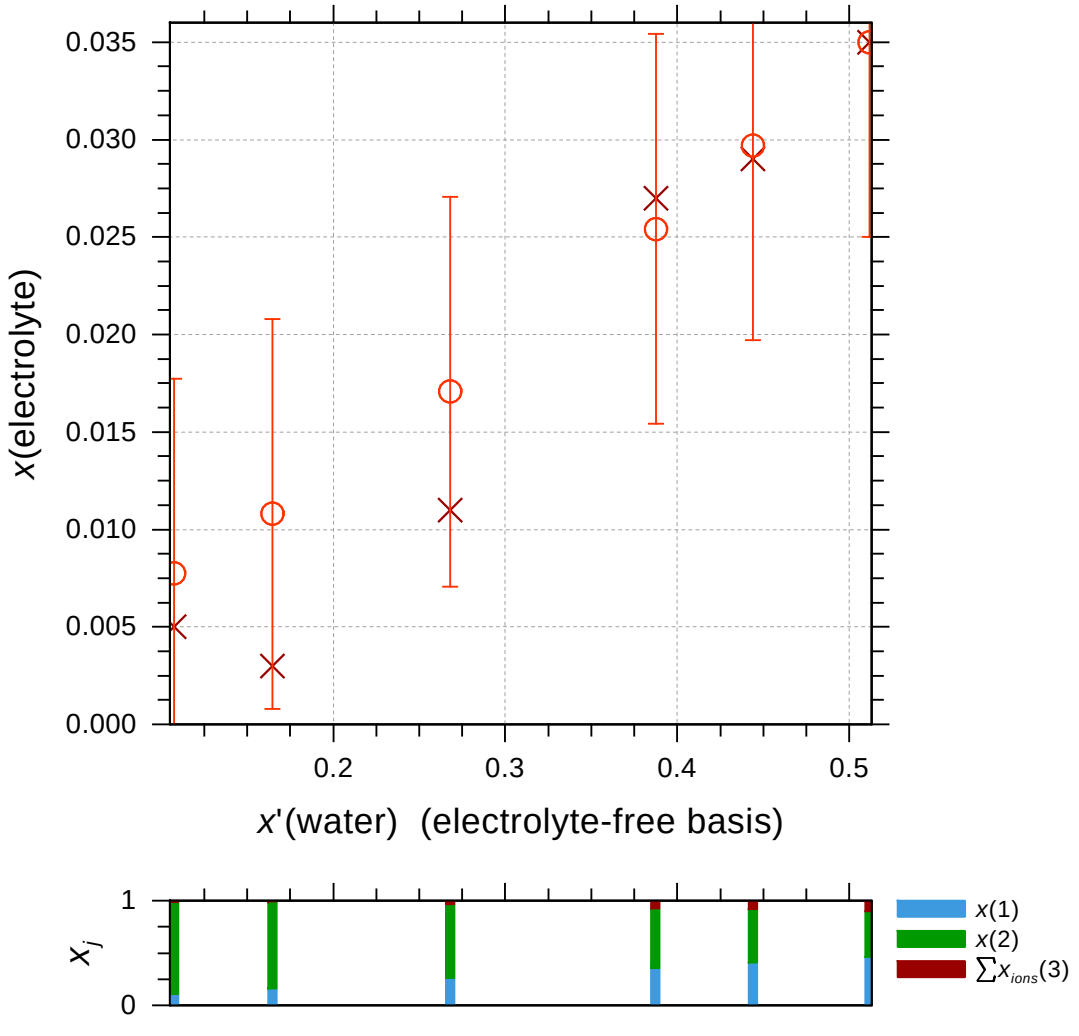


initial weighting of dataset:
$w^{init}(0370)$ = 0.010
dataset contribution to F_{obj}:
fval(0370) = 3.5888E+00
rel. contribution = 1.7066 %

Fig. S0094 (AIOMFAC_output_0371)

H_2O (1) + 2-Propanol (2) + $MgCl_2$ (3)

Temperature: 313 K

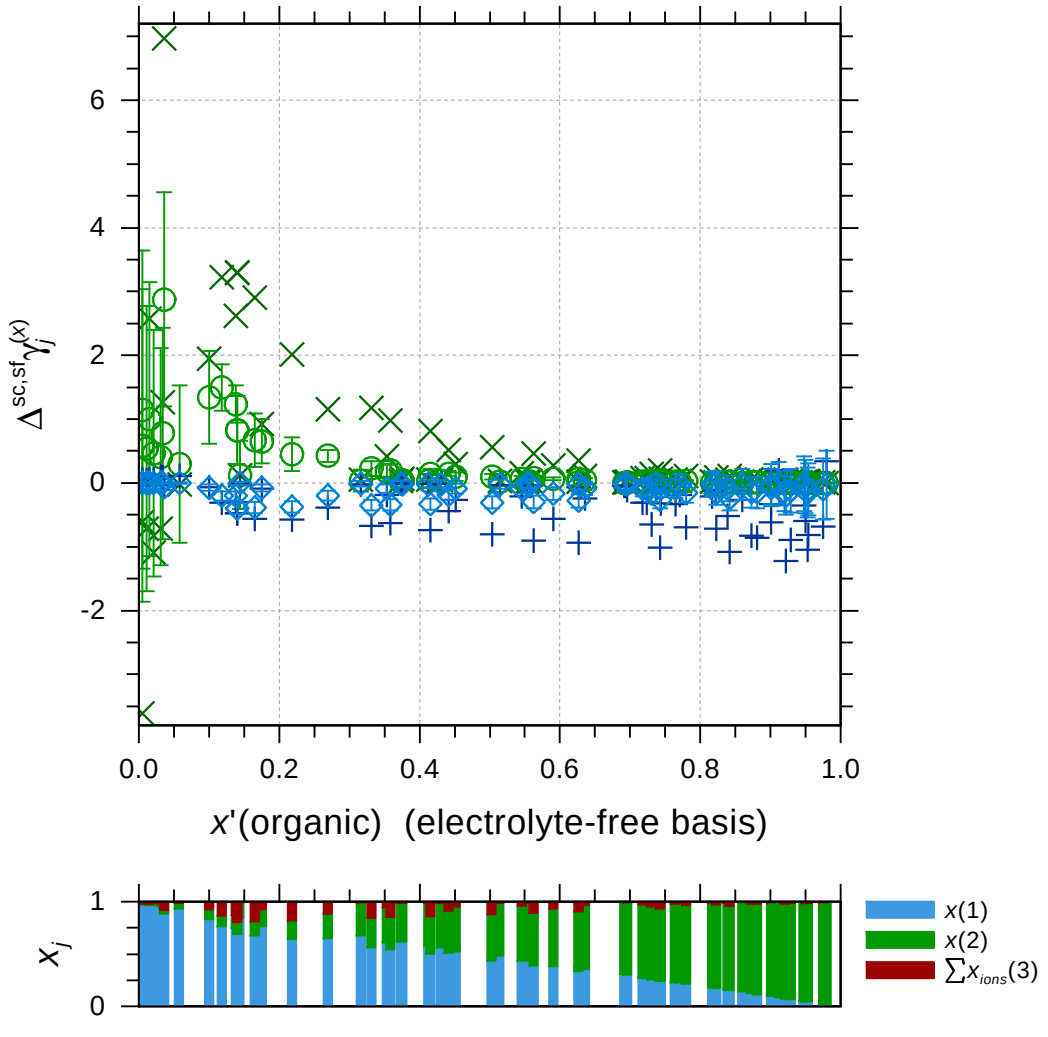


initial weighting of dataset:
w^{init}(0371) = 0.010
dataset contribution to F_{obj}:
fval(0371) = 4.7986E-03
rel. contribution = 0.0023 %

Fig. S0095 (AIOMFAC_output_0409)

H_2O (1) + 2-Propanol (2) + $MgCl_2$ (3)

Temperature range: 353 -- 371 K

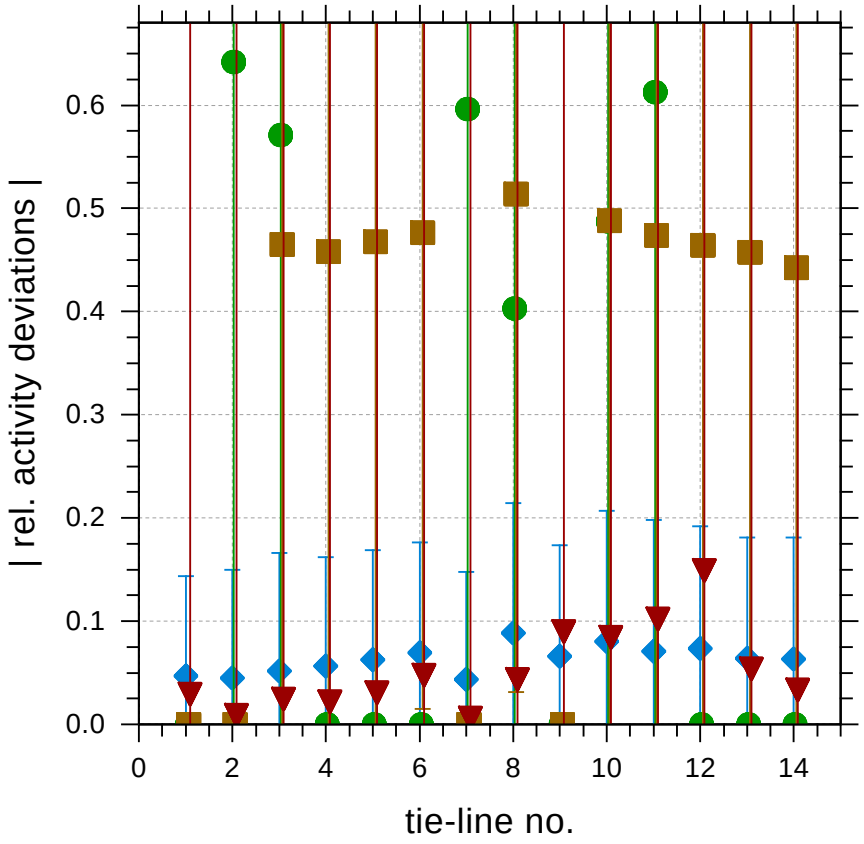


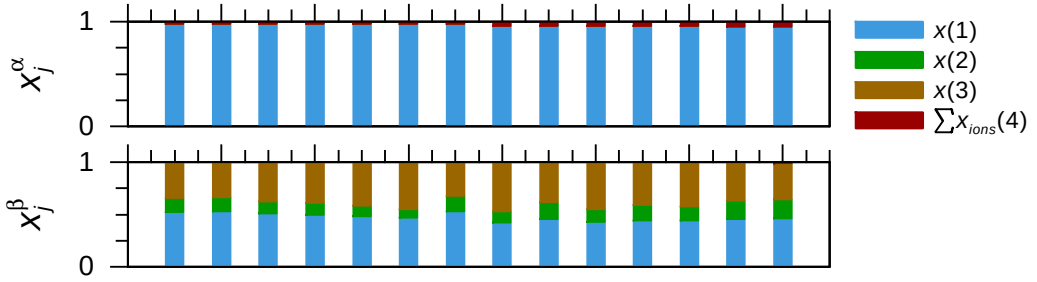
initial weighting of dataset:
$w^{init}(0409)$ = 0.500
dataset contribution to F_{obj}:
fval(0409) = 4.1062E-01
rel. contribution = 0.1953 %

Fig. S0096 (AIOMFAC_output_0425)

H_2O (1) + *tert*-Butanol (2) + 1-Butanol (3) + $MgCl_2$ (4)

Temperature: 293 K



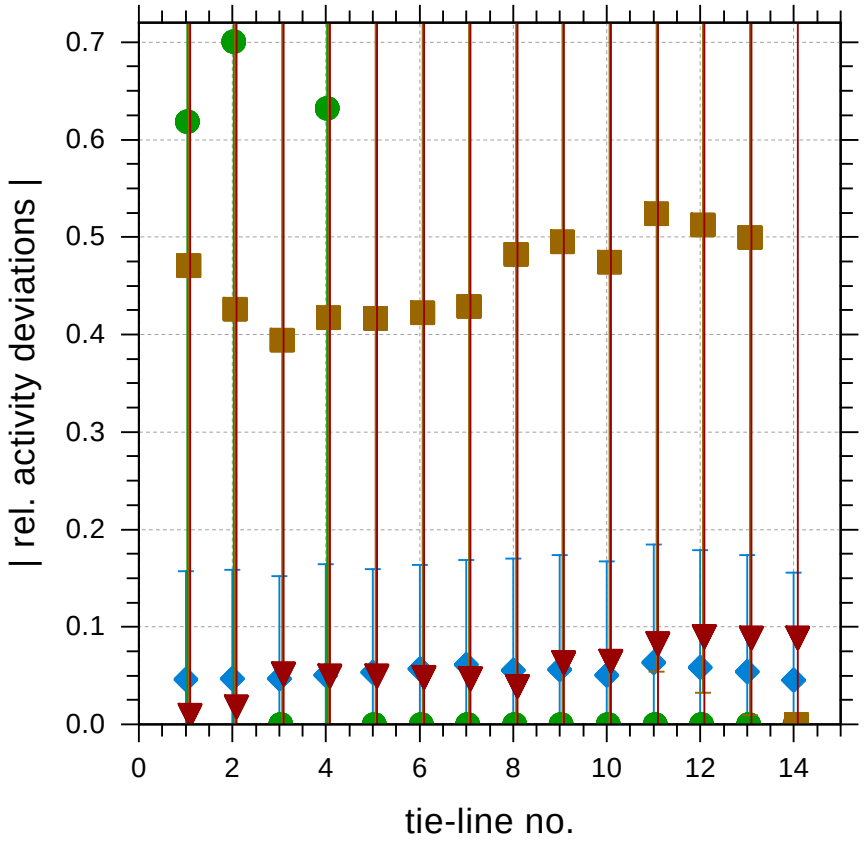


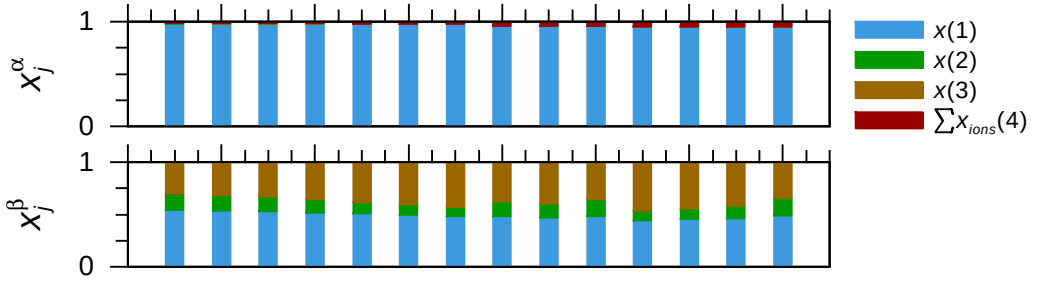
initial weighting of dataset:
$w^{init}(0425)$ = 1.000
dataset contribution to F_{obj}:
fval(0425) = 1.5014E+00
rel. contribution = 0.7140 %

Fig. S0097 (AIOMFAC_output_0426)

H_2O (1) + *tert*-Butanol (2) + 1-Butanol (3) + $MgCl_2$ (4)

Temperature: 313 K



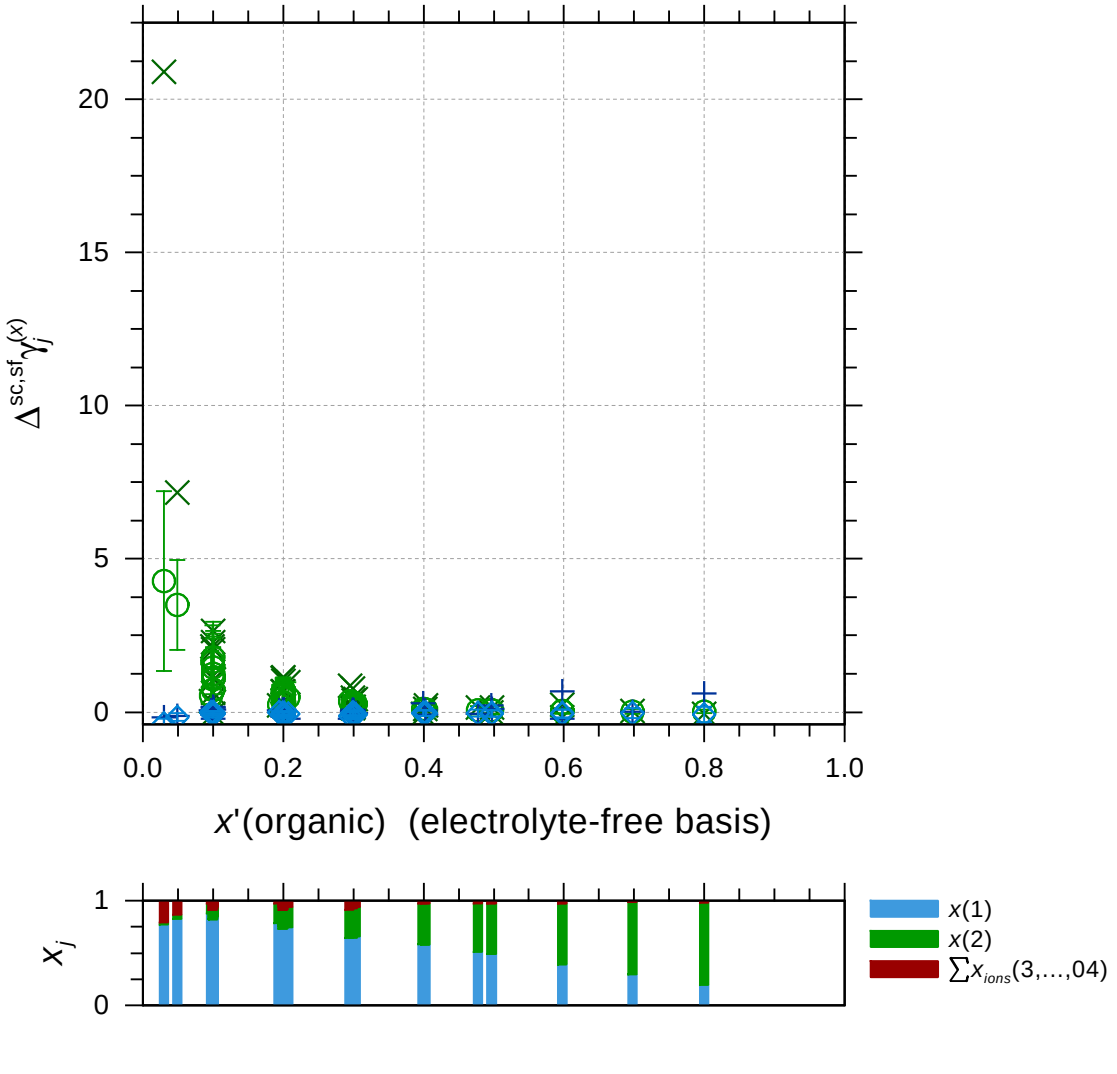


initial weighting of dataset:
$w^{init}(0426)$ = 0.800
dataset contribution to F_{obj}:
fval(0426) = 1.1783E+00
rel. contribution = 0.5603 %

Fig. S0098 (AIOMFAC_output_0368)

H_2O (1) + 2-Propanol (2) + $CaCl_2$ (3) + $MgCl_2$ (4)

Temperature: 313 K



initial weighting of dataset:

w^{init}(0368) = 0.500

dataset contribution to F_{obj}:

fval(0368) = 2.5261E-01

rel. contribution = 0.1201 %

Fig. S0100 (AIOMFAC_output_0374)

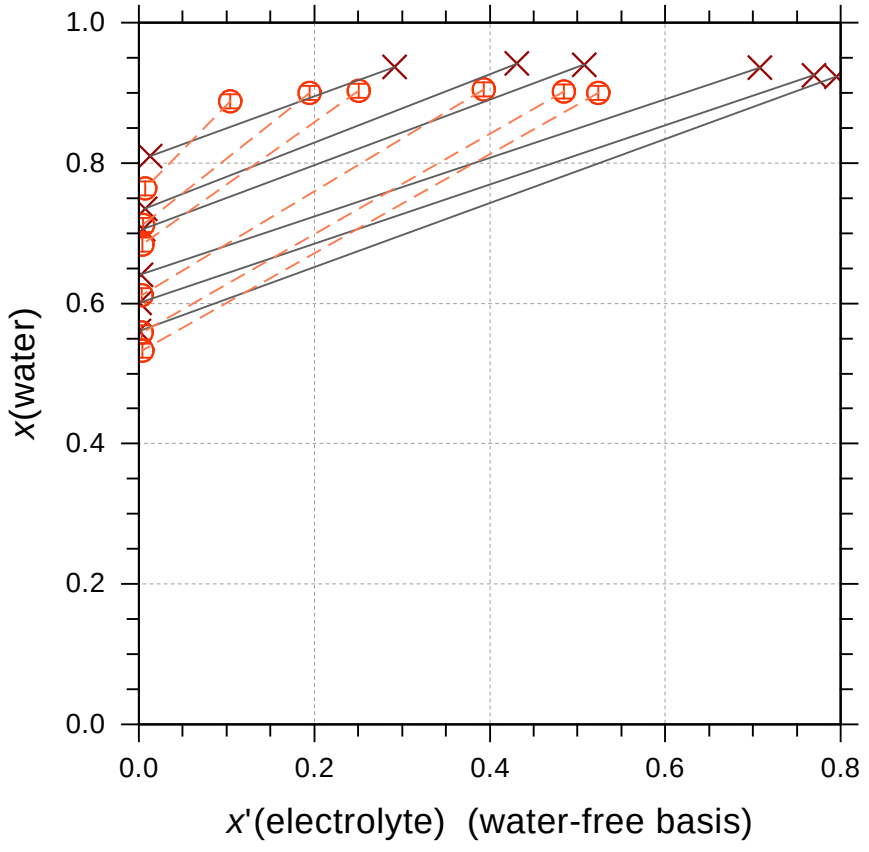
H_2O (1) + 1-Propanol (2) + $MgSO_4$ (3)

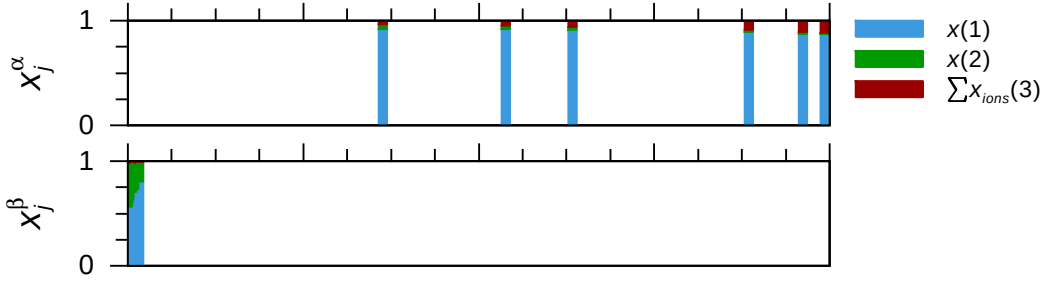
Temperature: 298 K

left y-axis:

× MgSO4+1-Propanol+Water_LLE_Zafarani-Moattar

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0374) = 1.000

dataset contribution to F_{obj}:

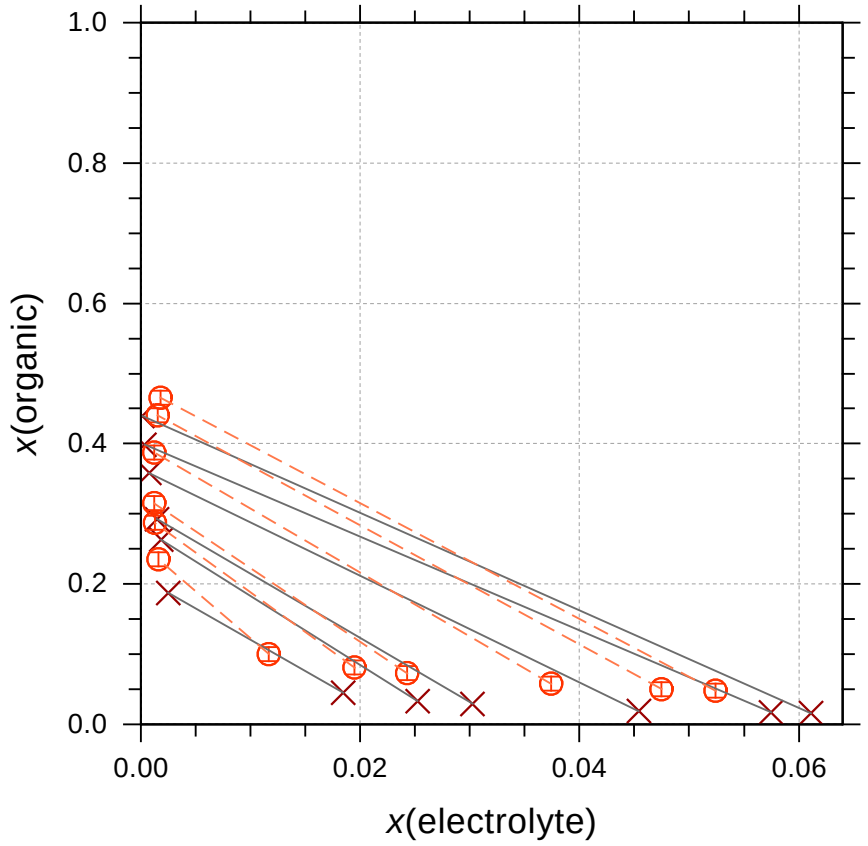
fval(0374) = 3.6255E-01

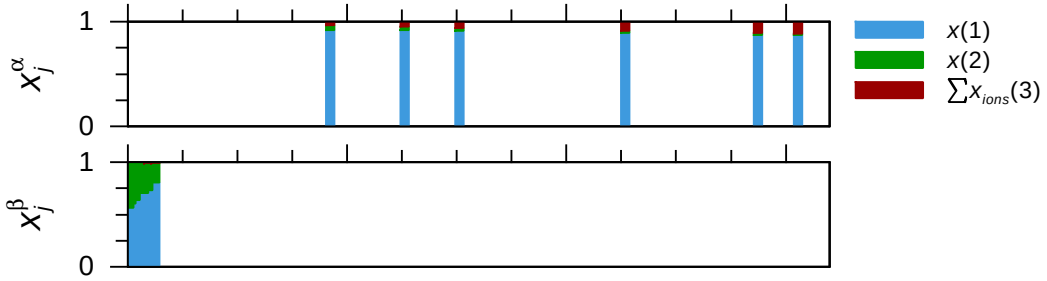
rel. contribution = 0.1724 %

Fig. S0100a (AIOMFAC_output_0374)

H_2O (1) + 1-Propanol (2) + $MgSO_4$ (3)

Temperature: 298 K



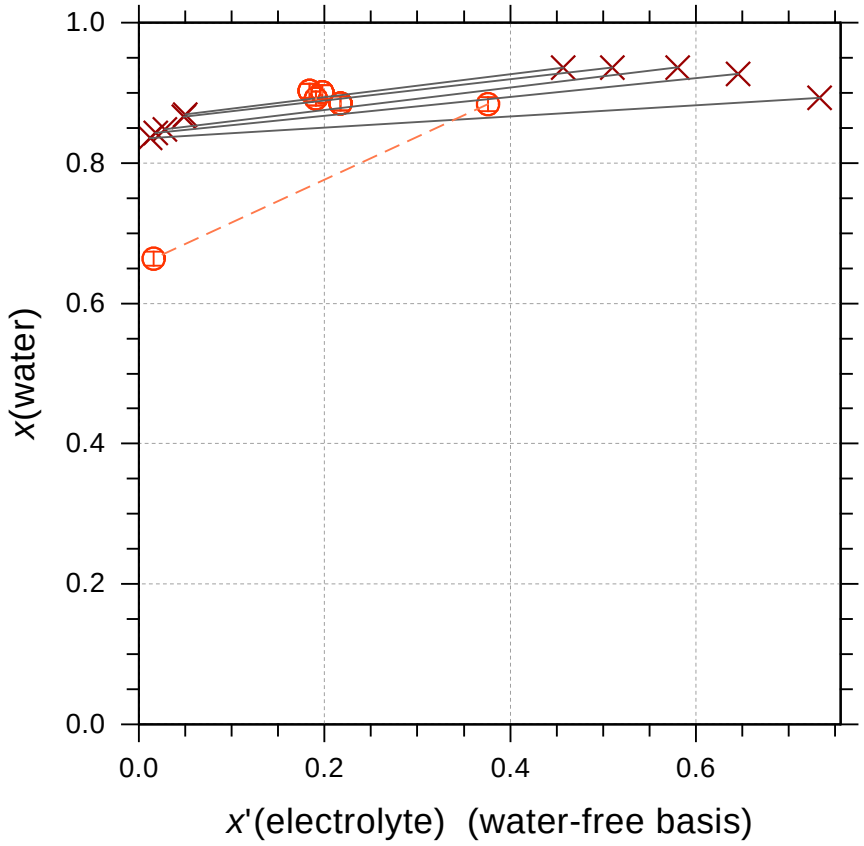


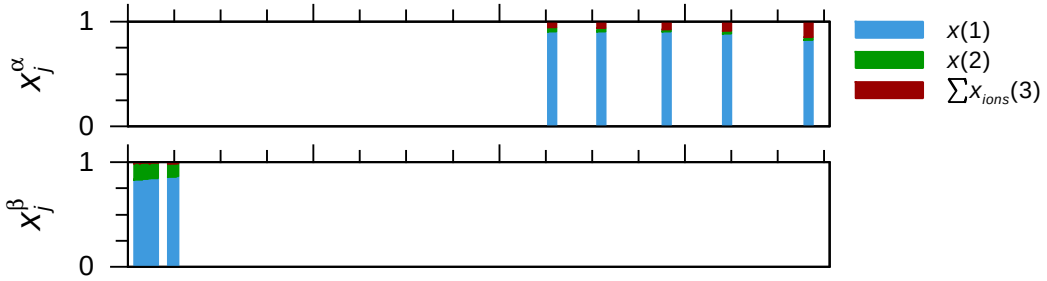
initial weighting of dataset:
$w^{init}(0374)$ = 1.000
dataset contribution to F_{obj}:
fval(0374) = 3.6255E-01
rel. contribution = 0.1724 %

Fig. S0101 (AIOMFAC_output_0375)

H_2O (1) + 2-Propanol (2) + $MgSO_4$ (3)

Temperature: 298 K





left y-axis:

× MgSO4+2-Propanol+Water_LLE_Zafarani-Moattar

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0375) = 0.500

dataset contribution to F_{obj}:

fval(0375) = 1.0556E+00

rel. contribution = 0.5020 %

Fig. S0101a (AIOMFAC_output_0375)

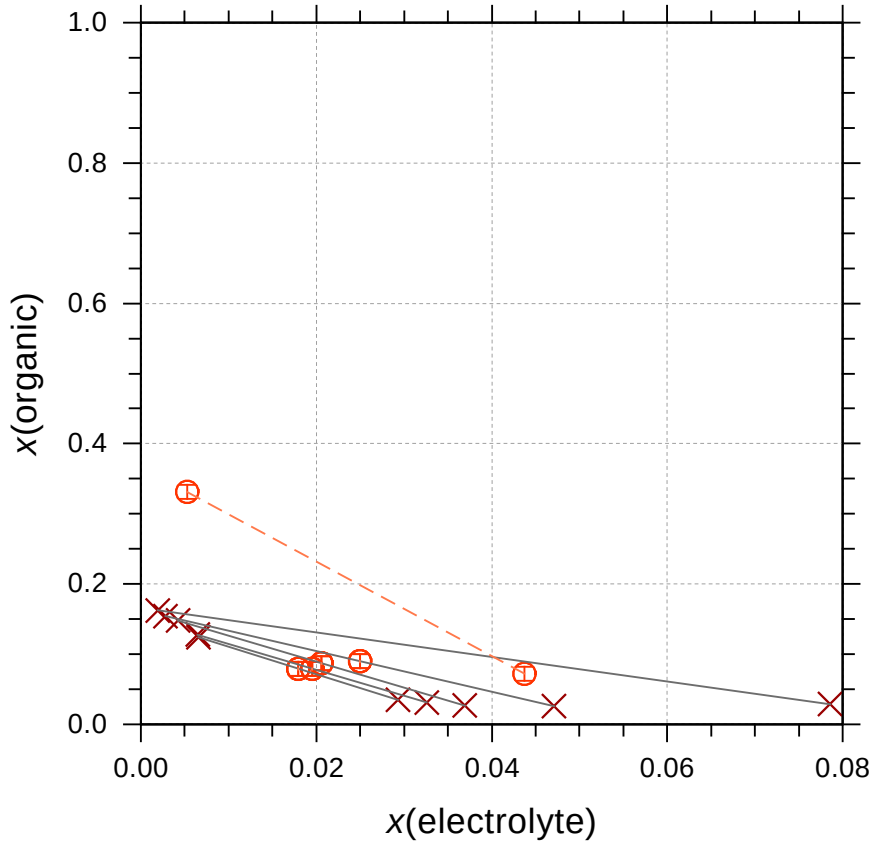
H_2O (1) + 2-Propanol (2) + $MgSO_4$ (3)

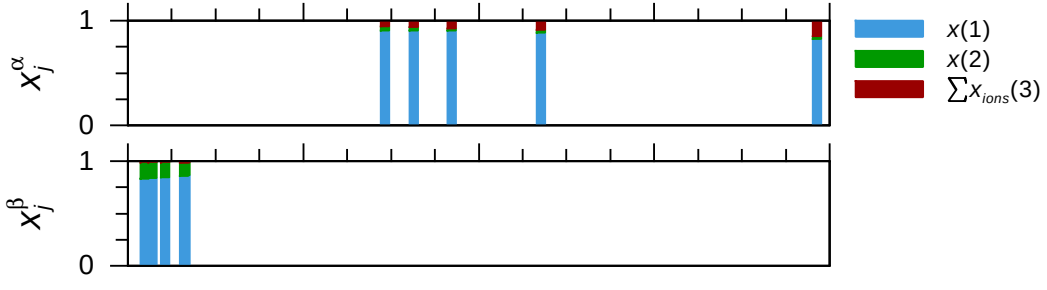
Temperature: 298 K

left y-axis:

× MgSO4+2-Propanol+Water_LLE_Zafarani-Moattar

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0375) = 0.500

dataset contribution to F_{obj}:

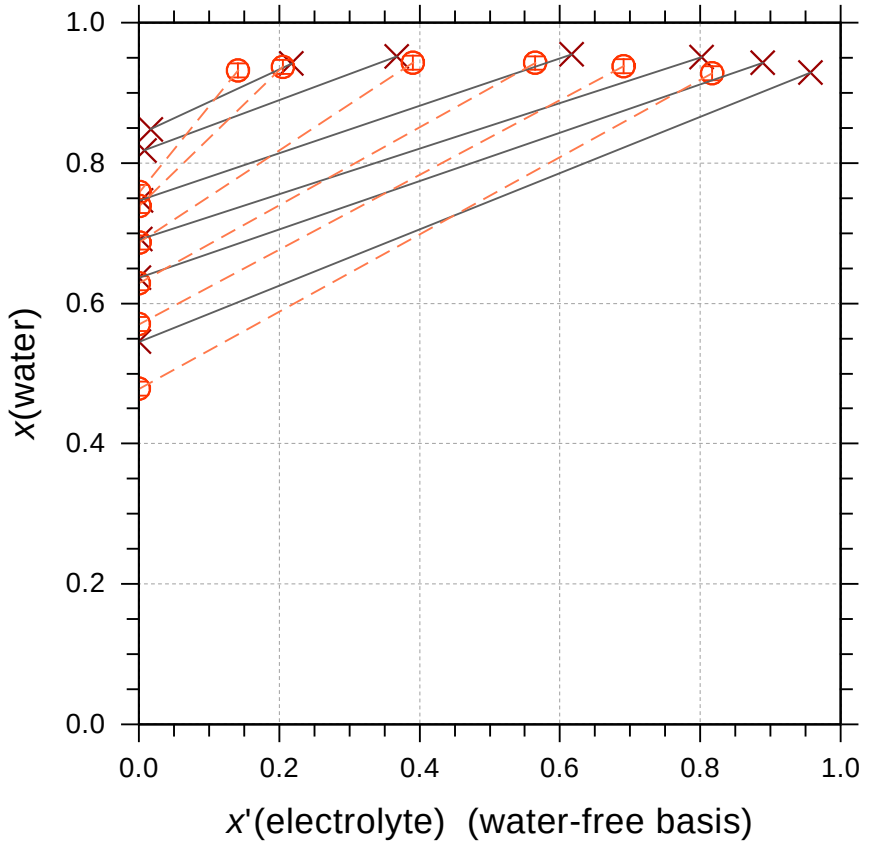
fval(0375) = 1.0556E+00

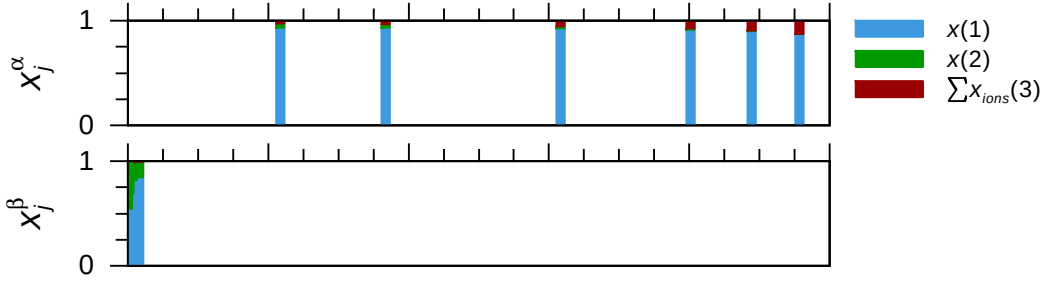
rel. contribution = 0.5020 %

Fig. S0102 (AIOMFAC_output_0376)

H_2O (1) + *tert*-Butanol (2) + $MgSO_4$ (3)

Temperature: 298 K





left y-axis:

× MgSO4+tert-Butanol+Water_LLE_Zafarani-Moattar

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0376) = 1.000

dataset contribution to F_{obj}:

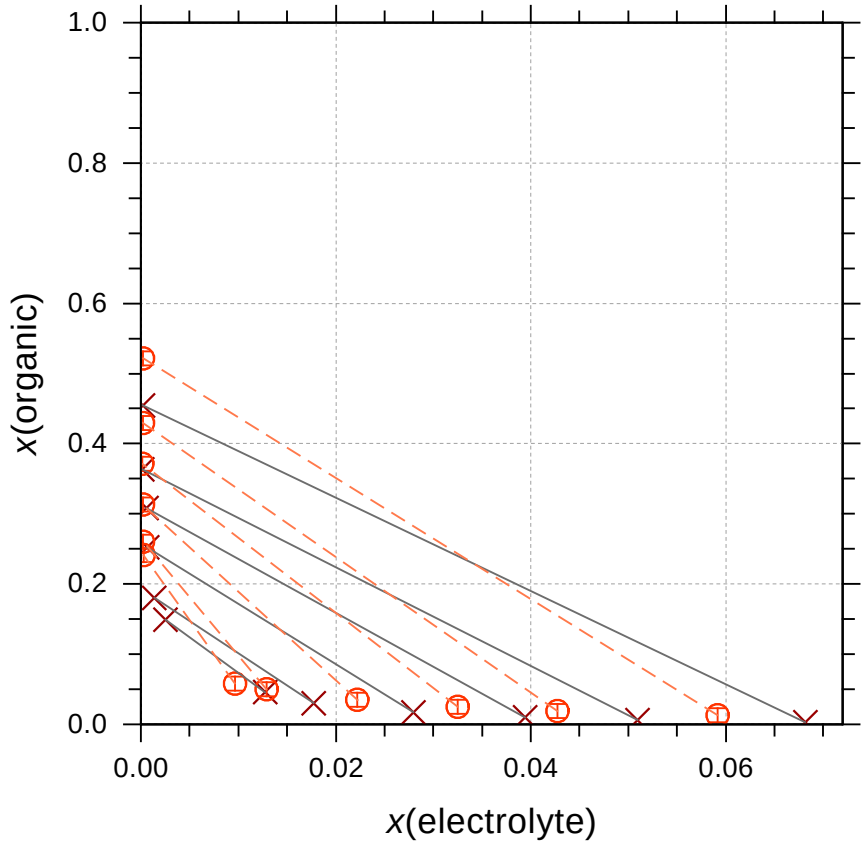
fval(0376) = 2.0430E-01

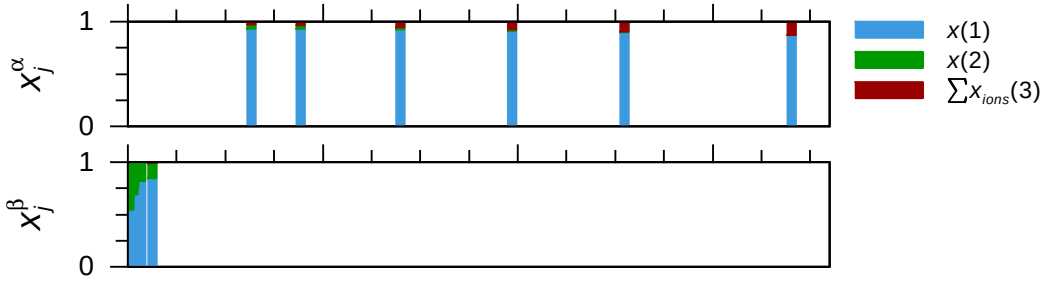
rel. contribution = 0.0972 %

Fig. S0102a (AIOMFAC_output_0376)

H_2O (1) + *tert*-Butanol (2) + $MgSO_4$ (3)

Temperature: 298 K





left y-axis:

× MgSO4+tert-Butanol+Water_LLE_Zafarani-Moattar

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0376) = 1.000

dataset contribution to F_{obj}:

fval(0376) = 2.0430E-01

rel. contribution = 0.0972 %

Fig. S0103 (AIOMFAC_output_1062)

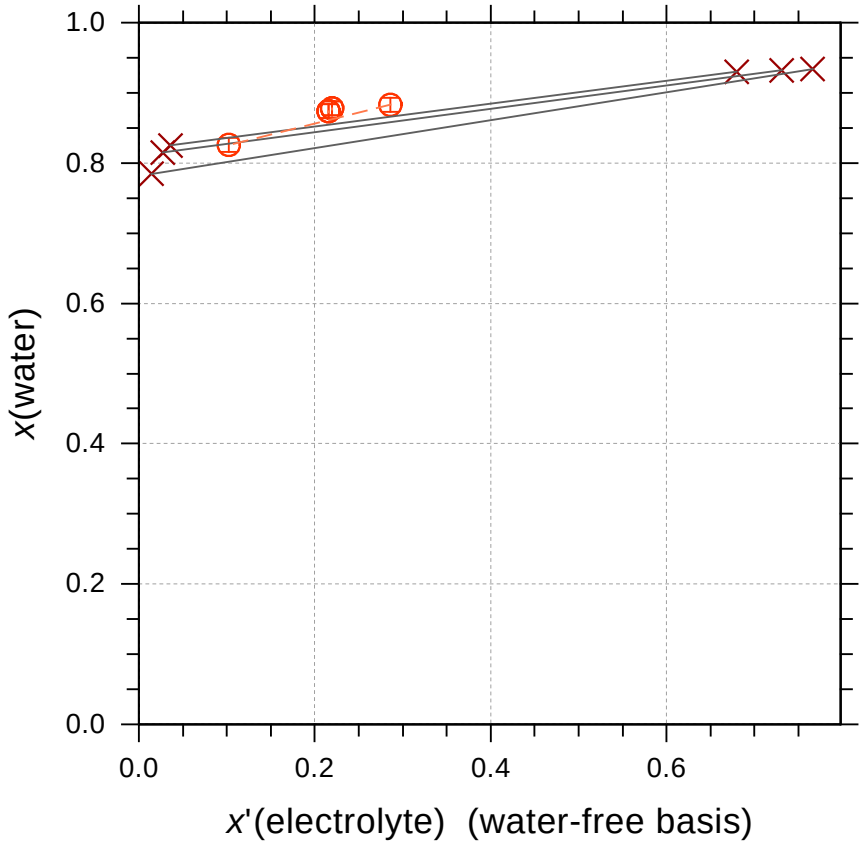
H_2O (1) + Ethanol (2) + Na_2SO_4 (3)

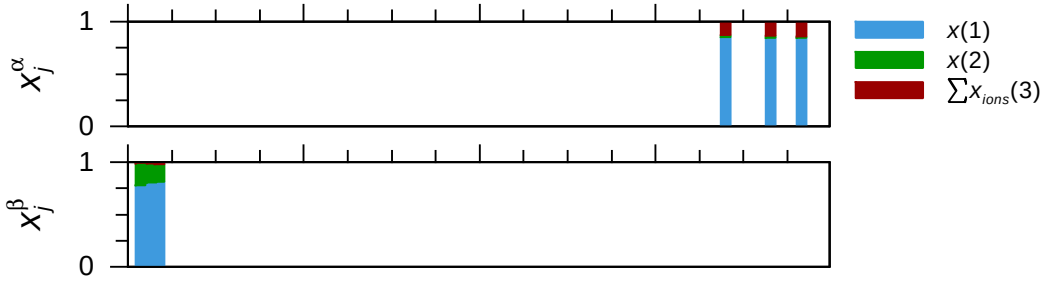
Temperature: 298 K

left y-axis:

× Na2SO4+Ethanol+Water_LLE_Greve

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(1062) = 1.000

dataset contribution to F_{obj}:

fval(1062) = 5.0896E-01

rel. contribution = 0.2420 %

Fig. S0103a (AIOMFAC_output_1062)

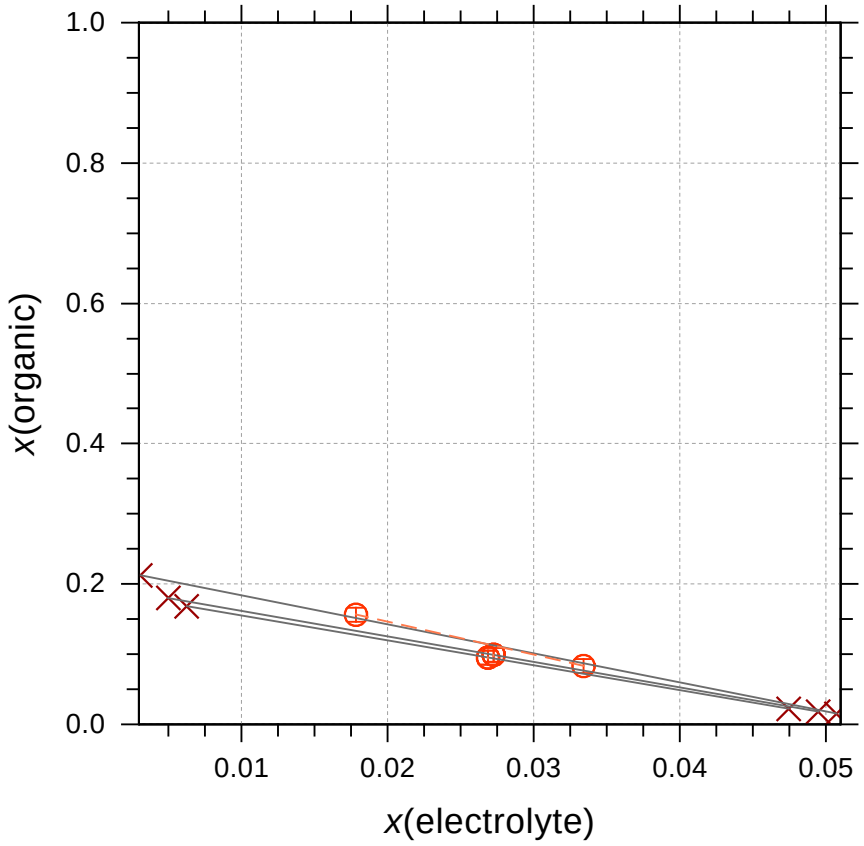
H_2O (1) + Ethanol (2) + Na_2SO_4 (3)

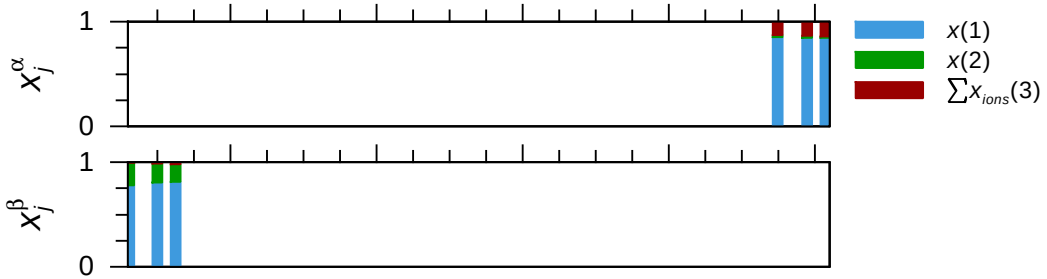
Temperature: 298 K

left y-axis:

× Na2SO4+Ethanol+Water_LLE_Greve

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(1062) = 1.000

dataset contribution to F_{obj}:

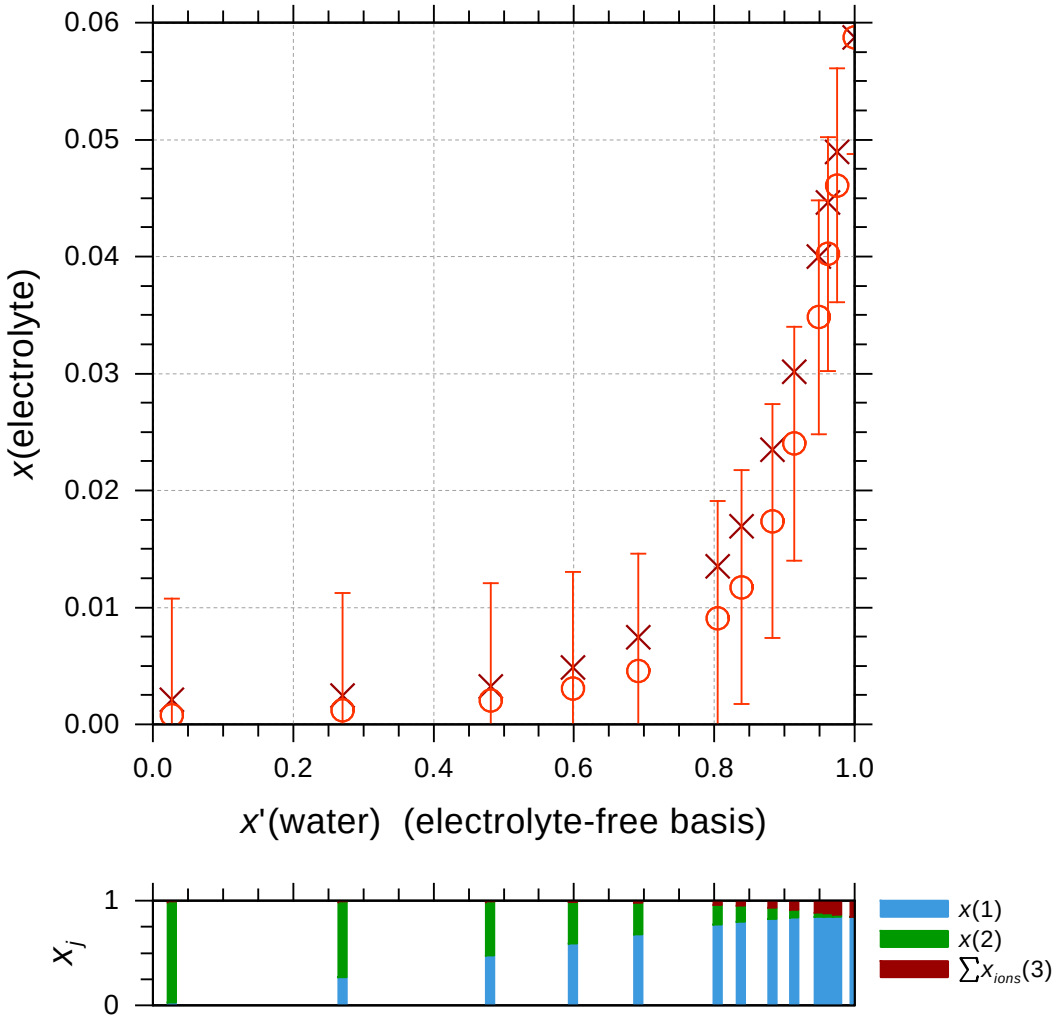
fval(1062) = 5.0896E-01

rel. contribution = 0.2420 %

Fig. S0104 (AIOMFAC_output_0082)

H_2O (1) + 1,2-Ethanediol (2) + Na_2SO_4 (3)

Temperature: 308 K

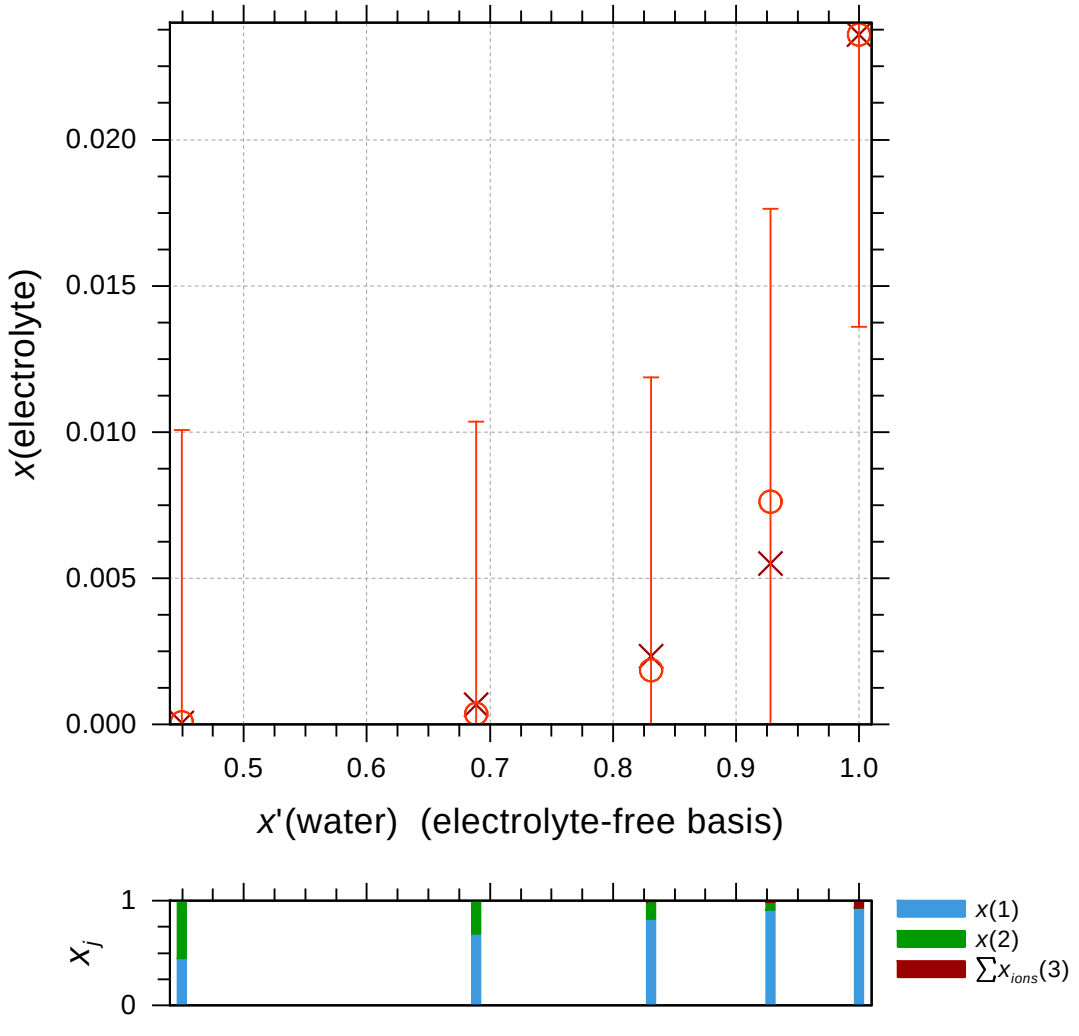


initial weighting of dataset:
w^{init}(0082) = 0.800
dataset contribution to F_{obj}:
fval(0082) = 1.3618E-01
rel. contribution = 0.0648 %

Fig. S0105 (AIOMFAC_output_0083)

H_2O (1) + 1-Propanol (2) + Na_2SO_4 (3)

Temperature: 293 K

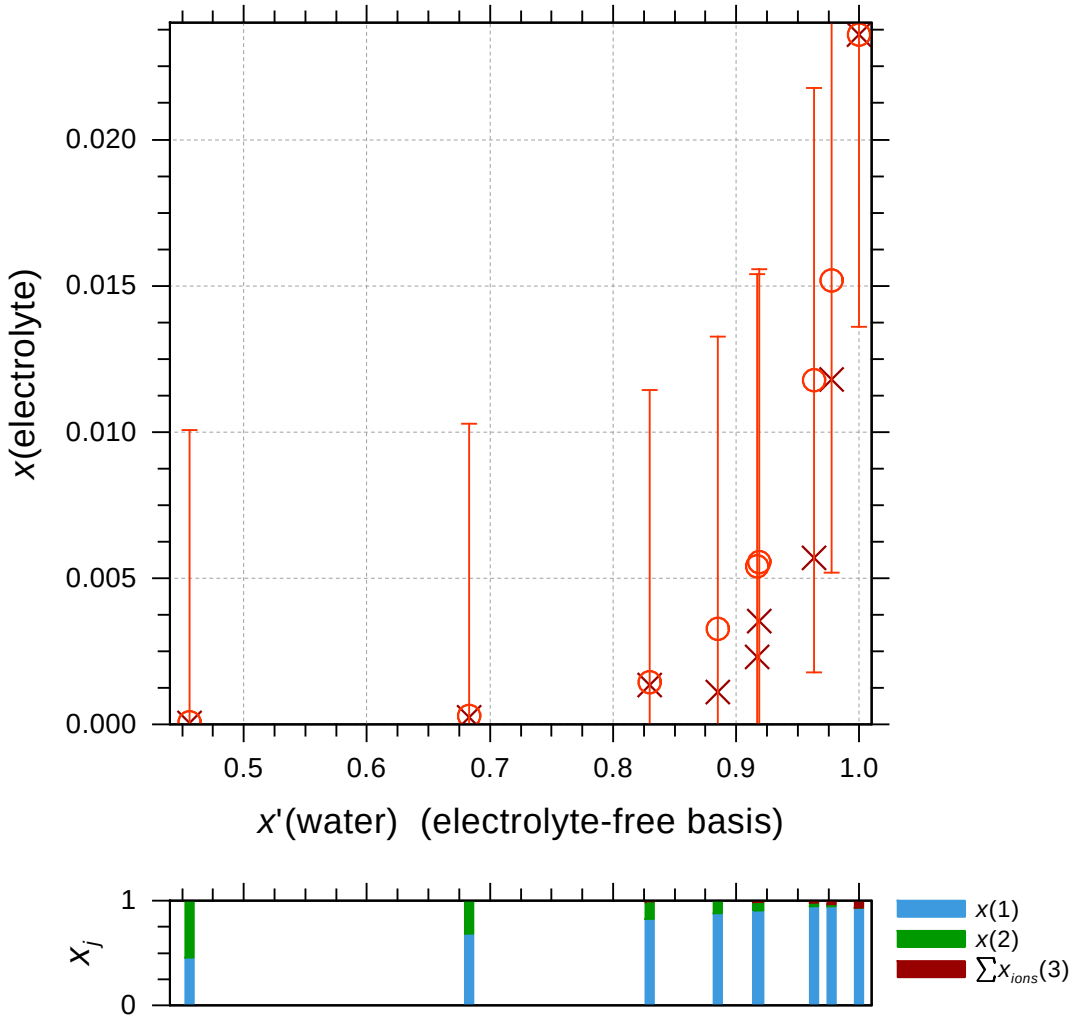


initial weighting of dataset:
w^{init}(0083) = 1.000
dataset contribution to F_{obj}:
fval(0083) = 2.1056E-02
rel. contribution = 0.0100 %

Fig. S0106 (AIOMFAC_output_0084)

H_2O (1) + 2-Propanol (2) + Na_2SO_4 (3)

Temperature: 293 K

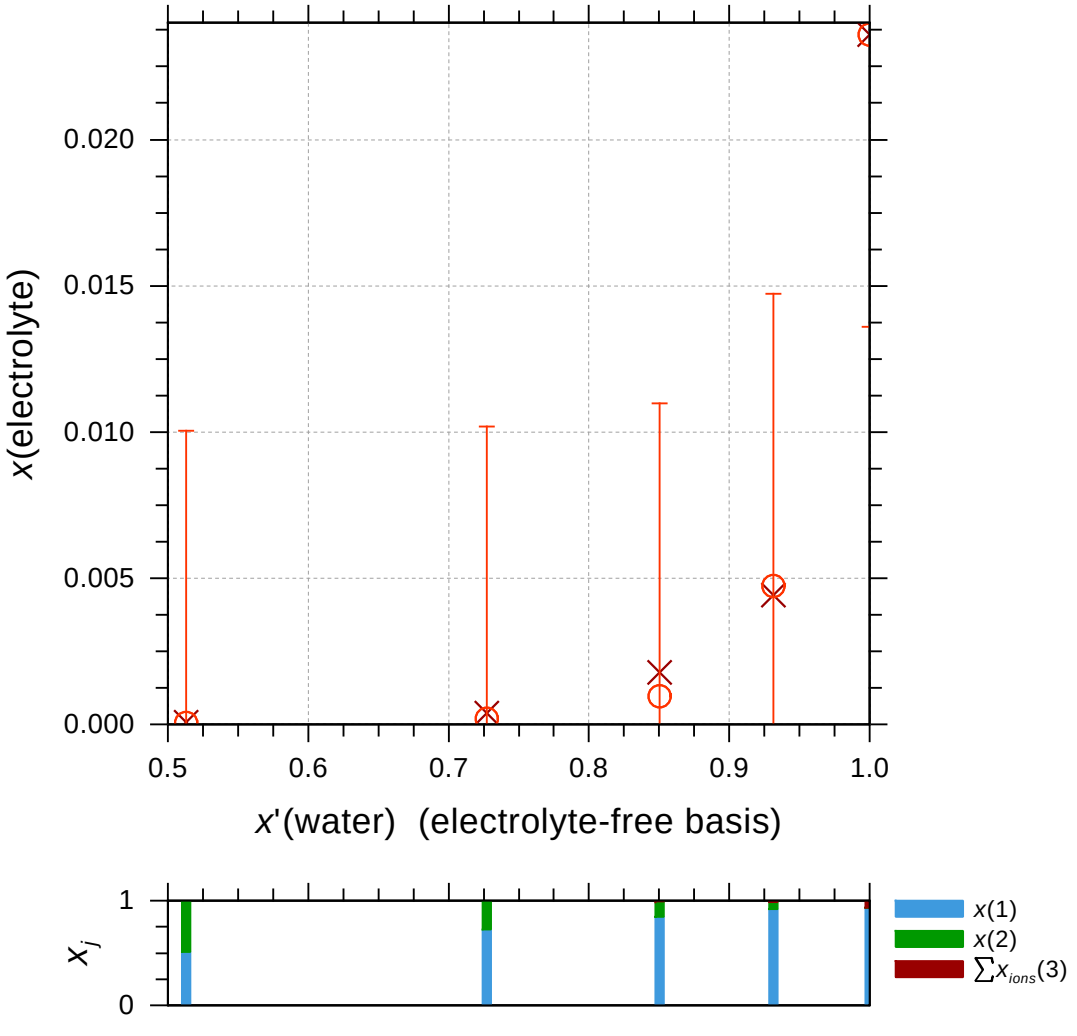


initial weighting of dataset:
w^{init}(0084) = 1.000
dataset contribution to F_{obj}:
fval(0084) = 2.9763E-01
rel. contribution = 0.1415 %

Fig. S0107 (AIOMFAC_output_0085)

H_2O (1) + *tert*-Butanol (2) + Na_2SO_4 (3)

Temperature: 293 K



initial weighting of dataset:
w^{init}(0085) = 1.000
dataset contribution to F_{obj}:
fval(0085) = 5.5768E-03
rel. contribution = 0.0027 %

Fig. S0108 (AIOMFAC_output_0086)

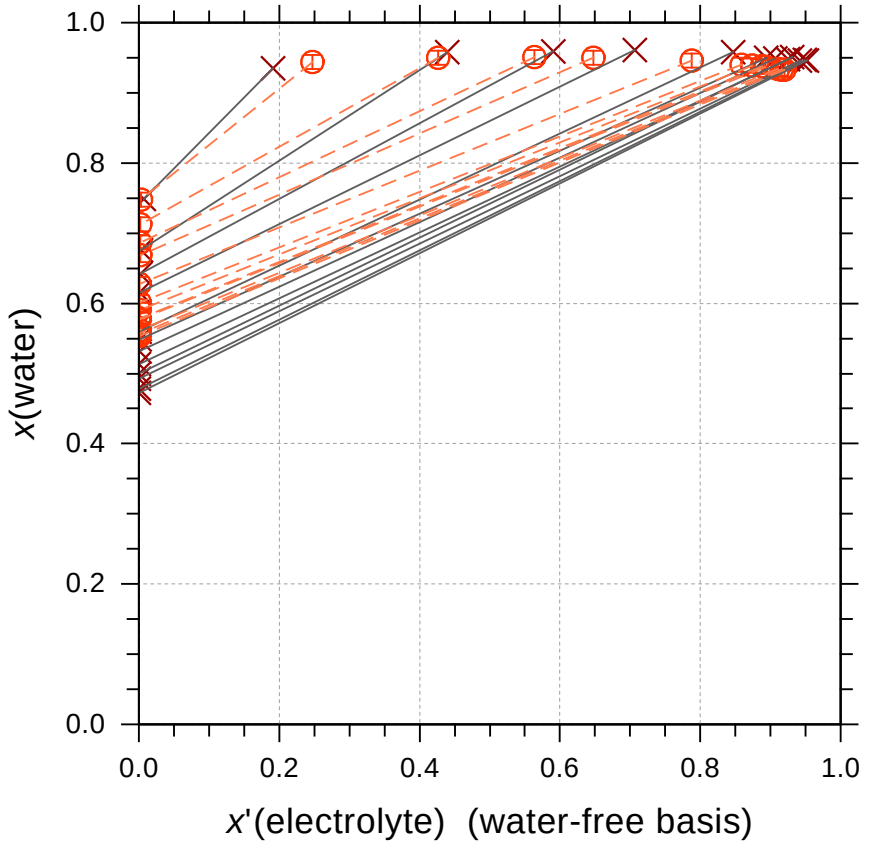
H_2O (1) + 1-Propanol (2) + Na_2SO_4 (3)

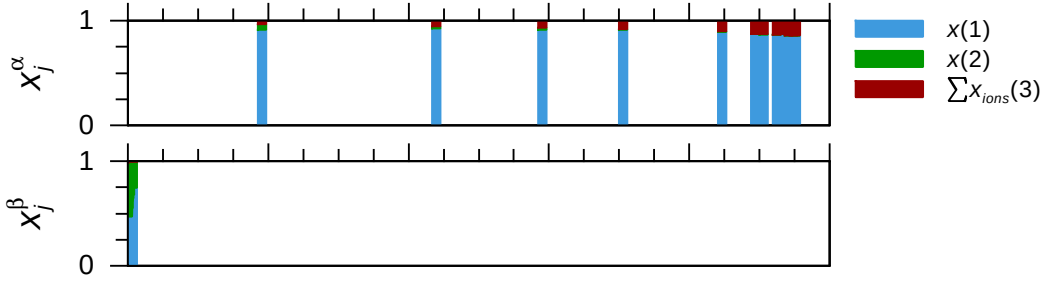
Temperature range: 297 -- 353 K

left y-axis:

× Na2SO4_1-PrOH_LLE_Brenner

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0086) = 1.000

dataset contribution to F_{obj}:

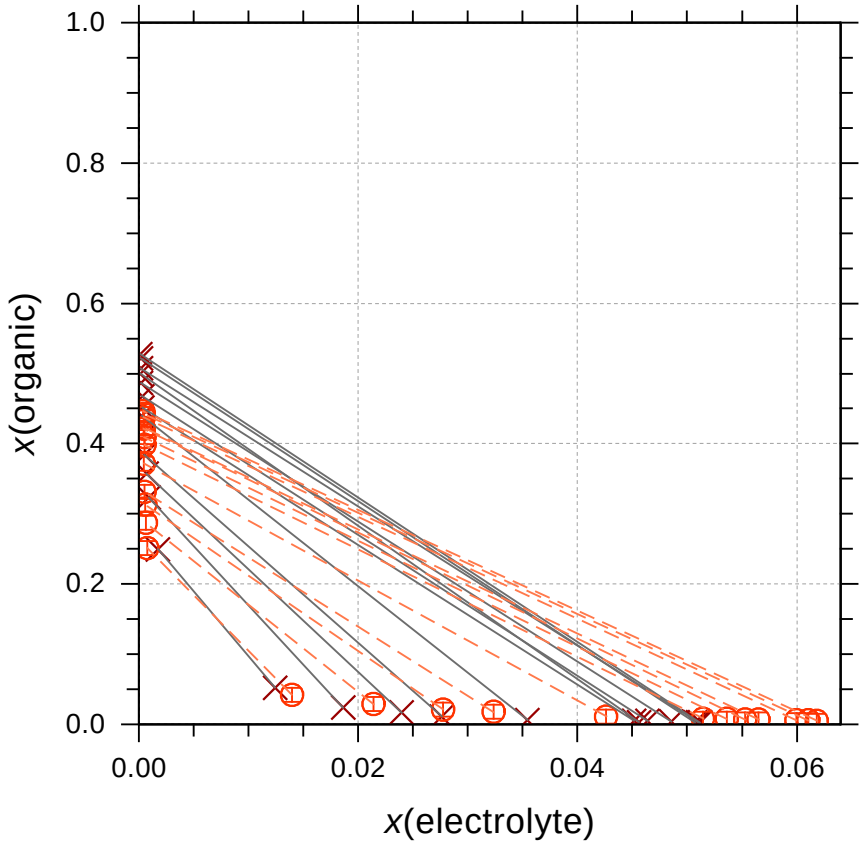
fval(0086) = 3.1132E-01

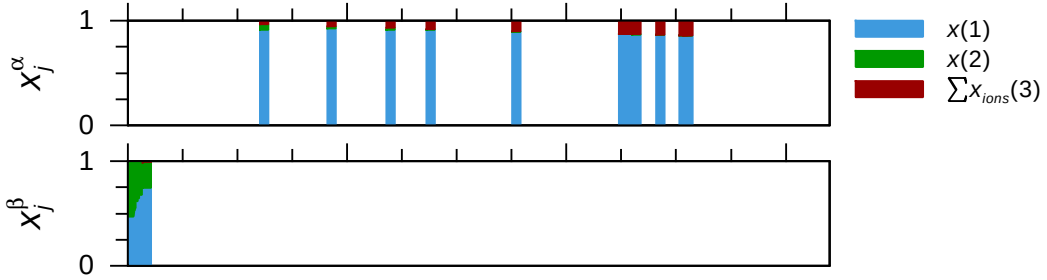
rel. contribution = 0.1480 %

Fig. S0108a (AIOMFAC_output_0086)

H_2O (1) + 1-Propanol (2) + Na_2SO_4 (3)

Temperature range: 297 -- 353 K





left y-axis:

× Na2SO4_1-PrOH_LLE_Brenner

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0086) = 1.000

dataset contribution to F_{obj}:

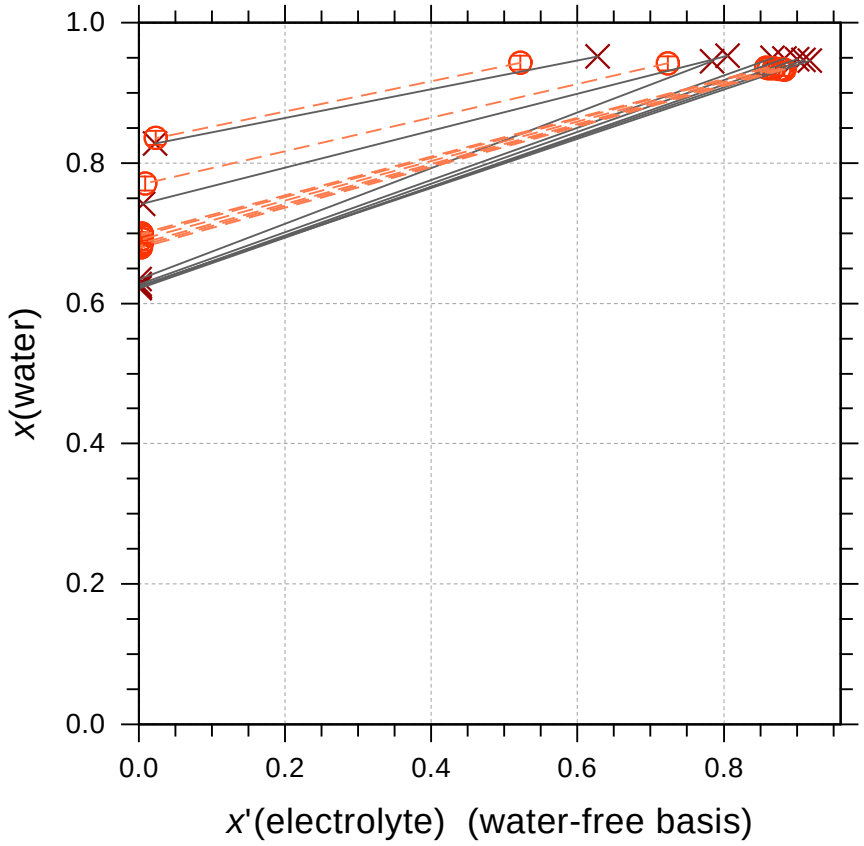
fval(0086) = 3.1132E-01

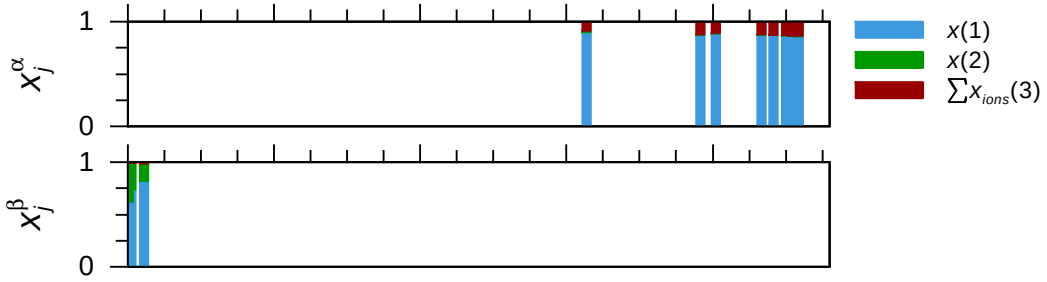
rel. contribution = 0.1480 %

Fig. S0109 (AIOMFAC_output_0087)

H_2O (1) + 2-Propanol (2) + Na_2SO_4 (3)

Temperature range: 302 -- 353 K





left y-axis:

× Na2SO4_2-PrOH_LLE_Brenner

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0087) = 1.000

dataset contribution to F_{obj}:

fval(0087) = 3.3614E-01

rel. contribution = 0.1598 %

Fig. S0109a (AIOMFAC_output_0087)

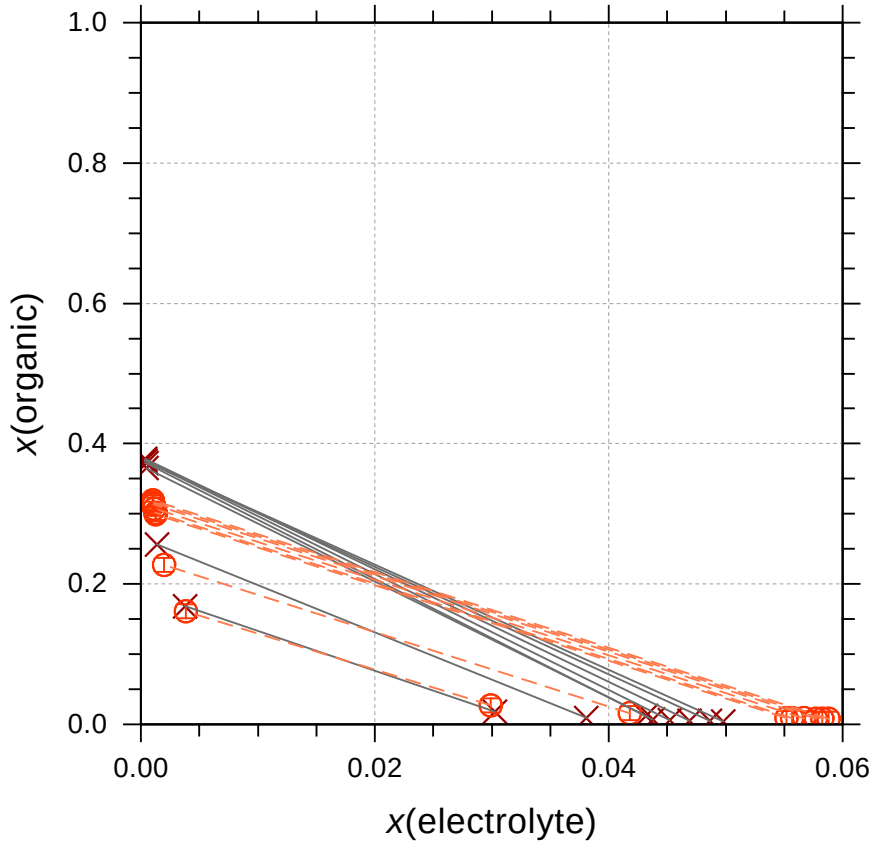
H_2O (1) + 2-Propanol (2) + Na_2SO_4 (3)

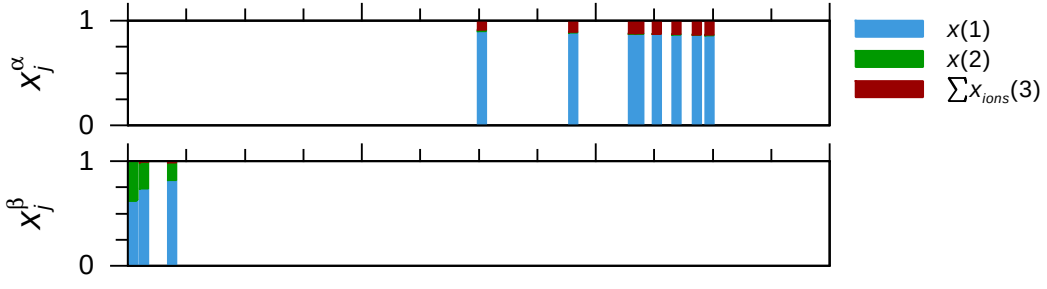
Temperature range: 302 -- 353 K

left y-axis:

× Na2SO4_2-PrOH_LLE_Brenner

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0087) = 1.000

dataset contribution to F_{obj}:

fval(0087) = 3.3614E-01

rel. contribution = 0.1598 %

Fig. S0110 (AIOMFAC_output_0088)

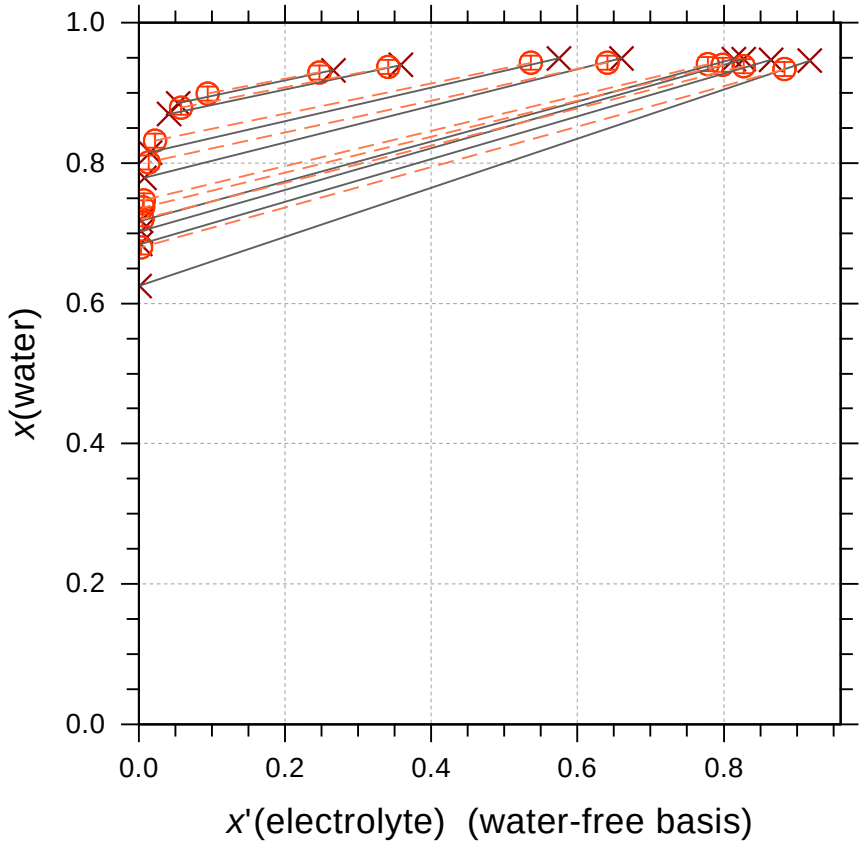
H_2O (1) + 2-Propanol (2) + Na_2SO_4 (3)

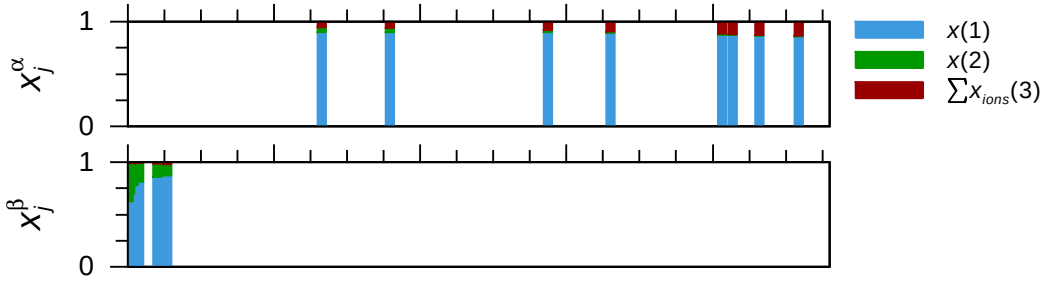
Temperature: 308 K

left y-axis:

× Na2SO4_2-PrOH_LLE_Lynn

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0088) = 1.000

dataset contribution to F_{obj}:

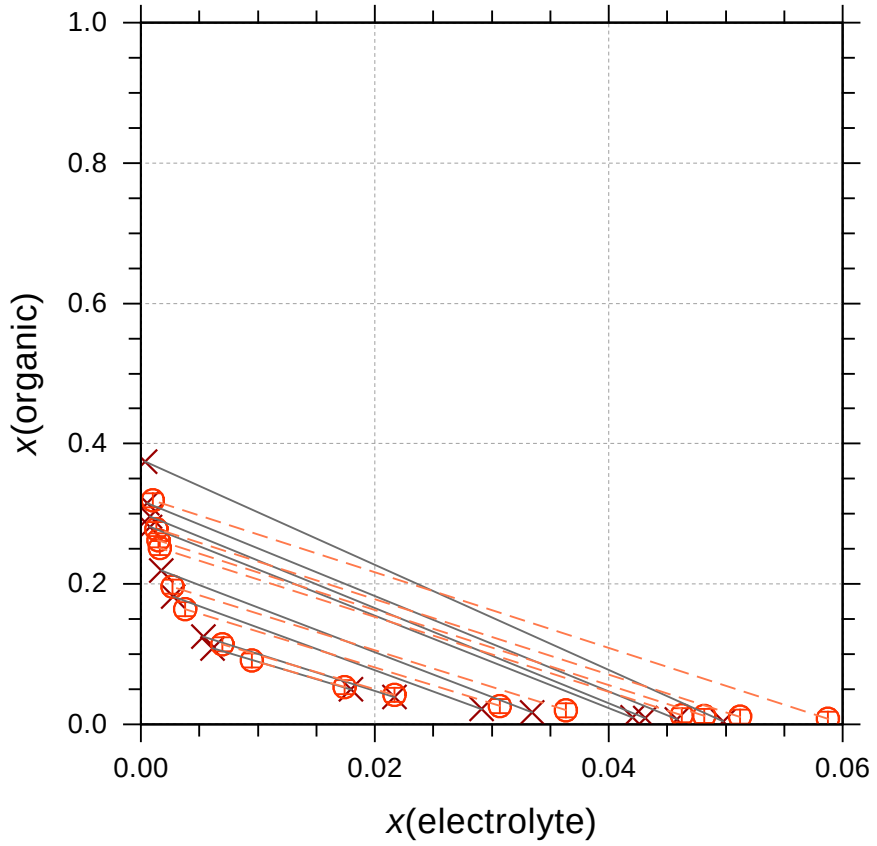
fval(0088) = 1.4222E-01

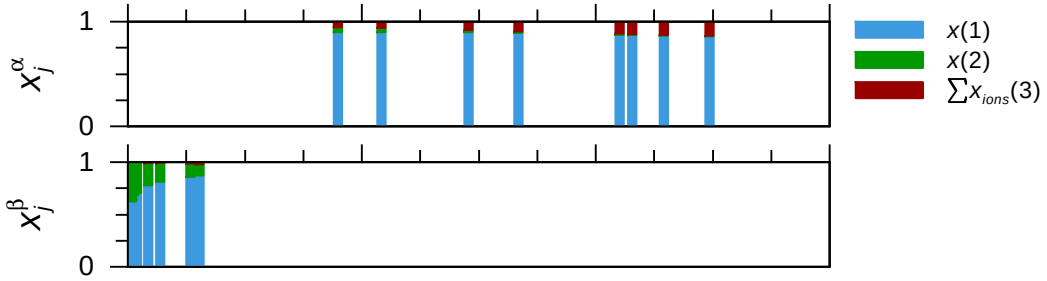
rel. contribution = 0.0676 %

Fig. S0110a (AIOMFAC_output_0088)

H_2O (1) + 2-Propanol (2) + Na_2SO_4 (3)

Temperature: 308 K



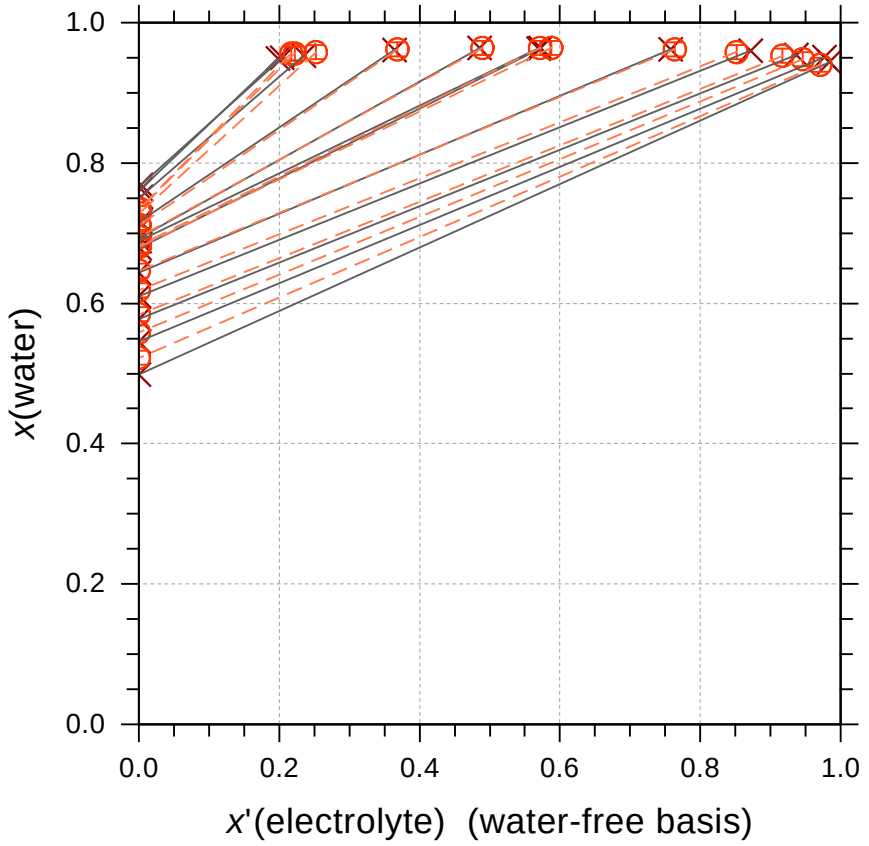


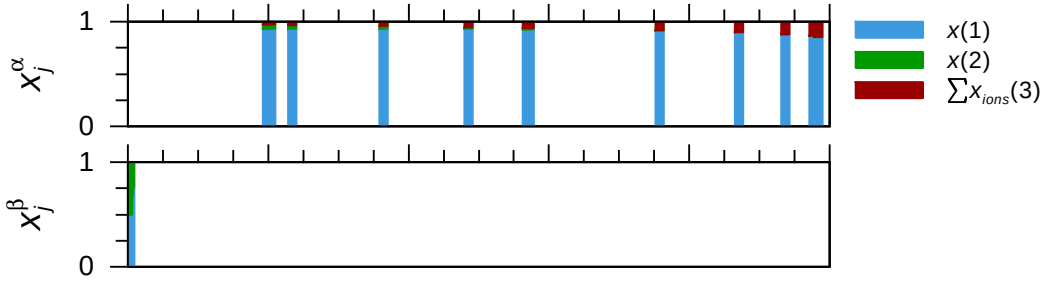
initial weighting of dataset:
w^{init}(0088) = 1.000
dataset contribution to F_{obj}:
fval(0088) = 1.4222E-01
rel. contribution = 0.0676 %

Fig. S0111 (AIOMFAC_output_0089)

H_2O (1) + *tert*-Butanol (2) + Na_2SO_4 (3)

Temperature: 308 K





left y-axis:

× Na2SO4_tert-BuOH_LLE_Lynn

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0089) = 1.000

dataset contribution to F_{obj}:

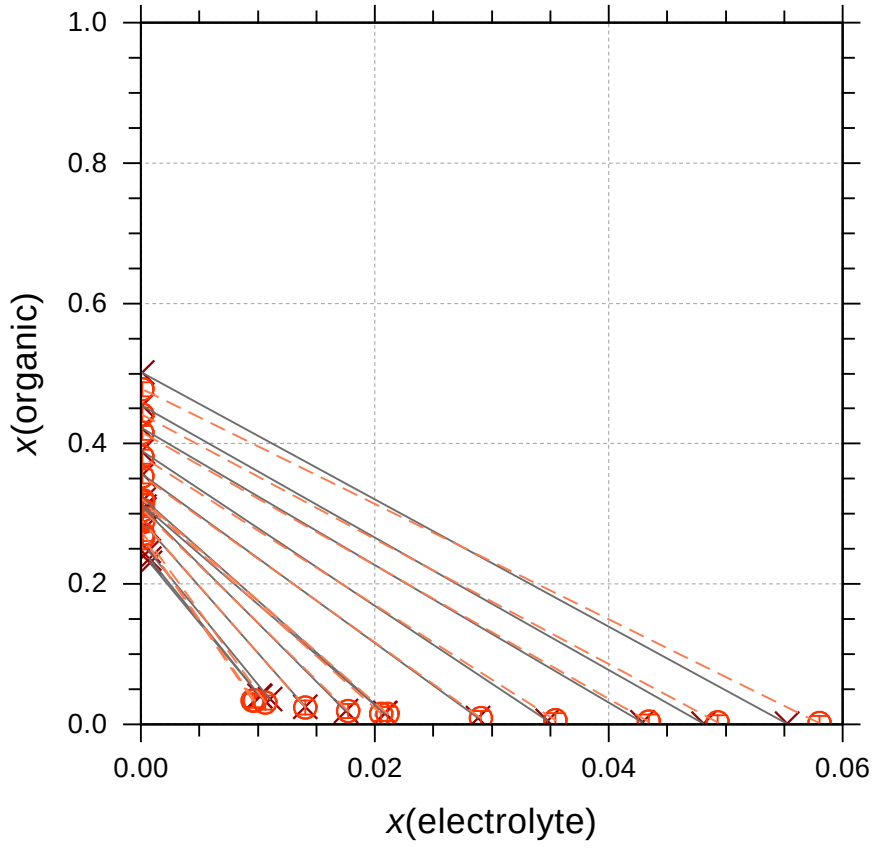
fval(0089) = 1.9553E-02

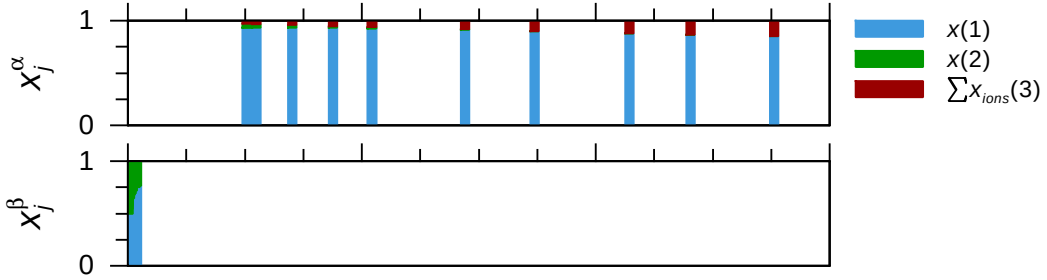
rel. contribution = 0.0093 %

Fig. S0111a (AIOMFAC_output_0089)

H_2O (1) + *tert*-Butanol (2) + Na_2SO_4 (3)

Temperature: 308 K





initial weighting of dataset:
$w^{init}(0089)$ = 1.000
dataset contribution to F_{obj}:
fval(0089) = 1.9553E-02
rel. contribution = 0.0093 %

Fig. S0112 (AIOMFAC_output_0090)

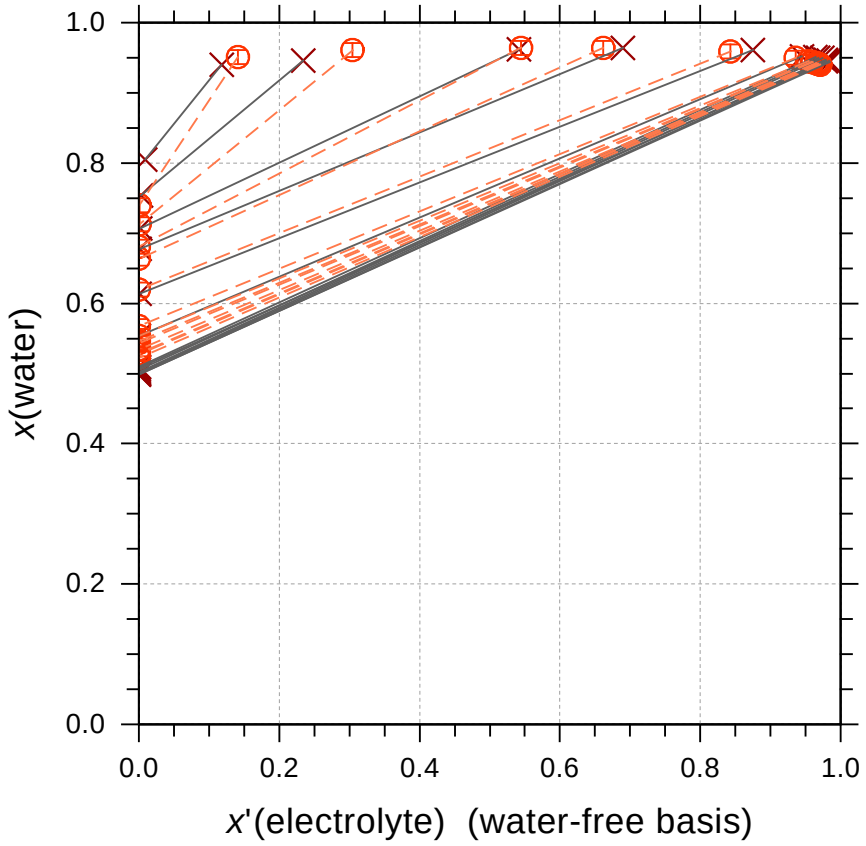
H_2O (1) + *tert*-Butanol (2) + Na_2SO_4 (3)

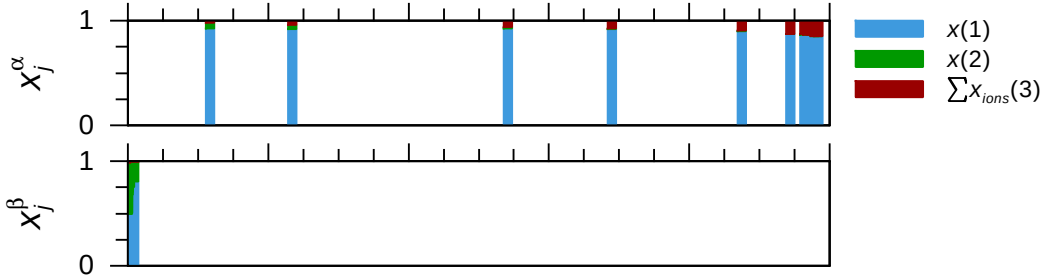
Temperature range: 296 -- 353 K

left y-axis:

× Na2SO4_tert-BuOH_LLE_Brenner

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0090)$ = 0.100

dataset contribution to F_{obj}:

fval(0090) = 4.7609E-03

rel. contribution = 0.0023 %

Fig. S0112a (AIOMFAC_output_0090)

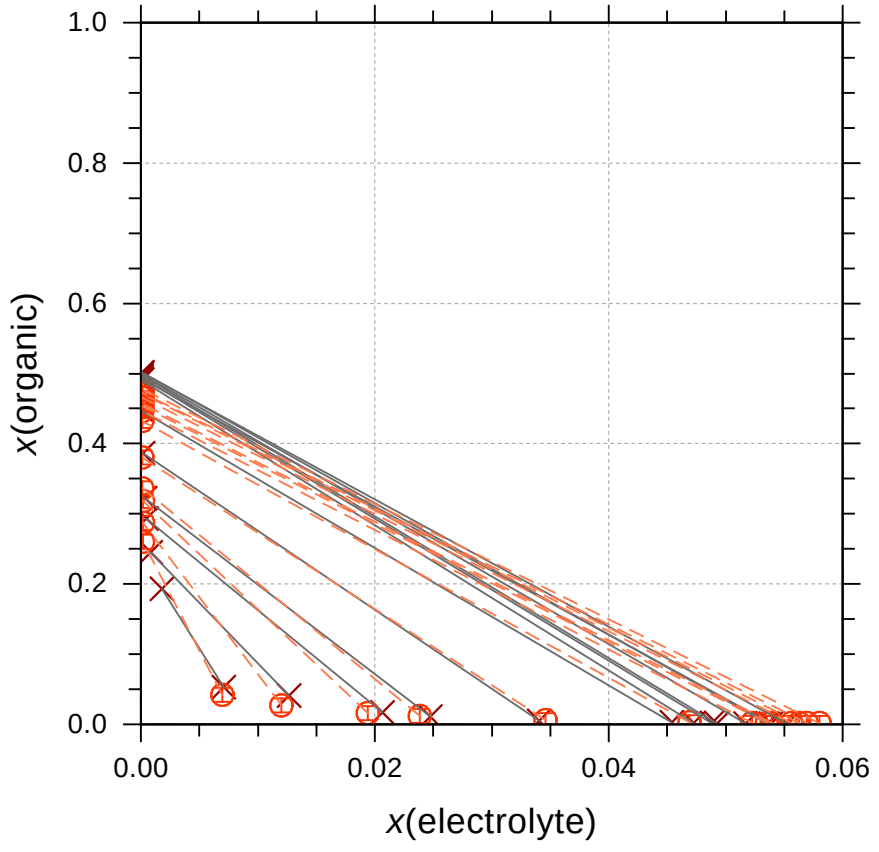
H_2O (1) + *tert*-Butanol (2) + Na_2SO_4 (3)

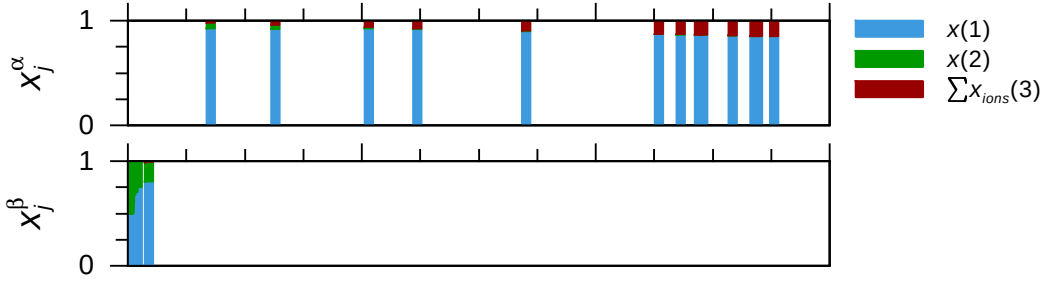
Temperature range: 296 -- 353 K

left y-axis:

× Na2SO4_tert-BuOH_LLE_Brenner

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0090)$ = 0.100

dataset contribution to F_{obj}:

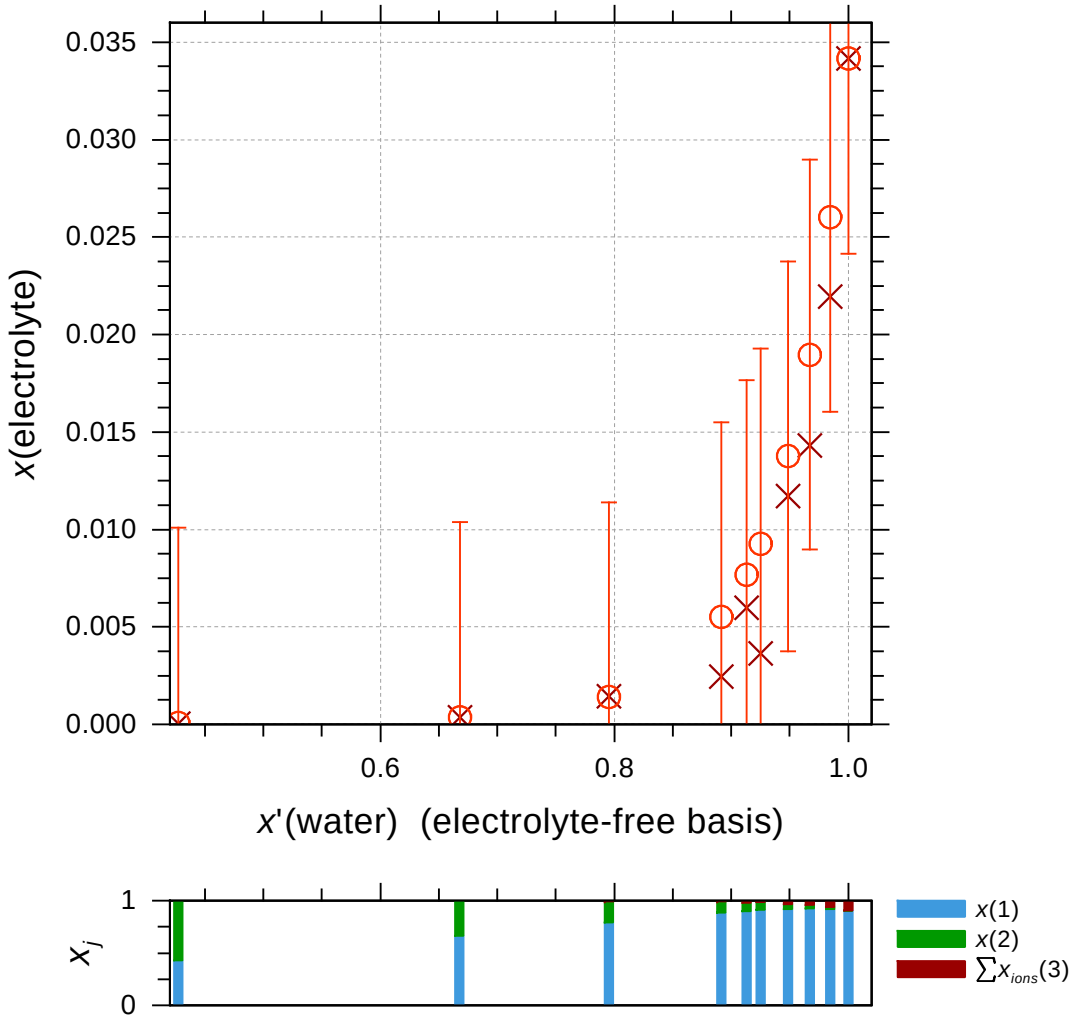
fval(0090) = 4.7609E-03

rel. contribution = 0.0023 %

Fig. S0113 (AIOMFAC_output_0110)

H_2O (1) + 2-Propanol (2) + Na_2SO_4 (3)

Temperature: 298 K

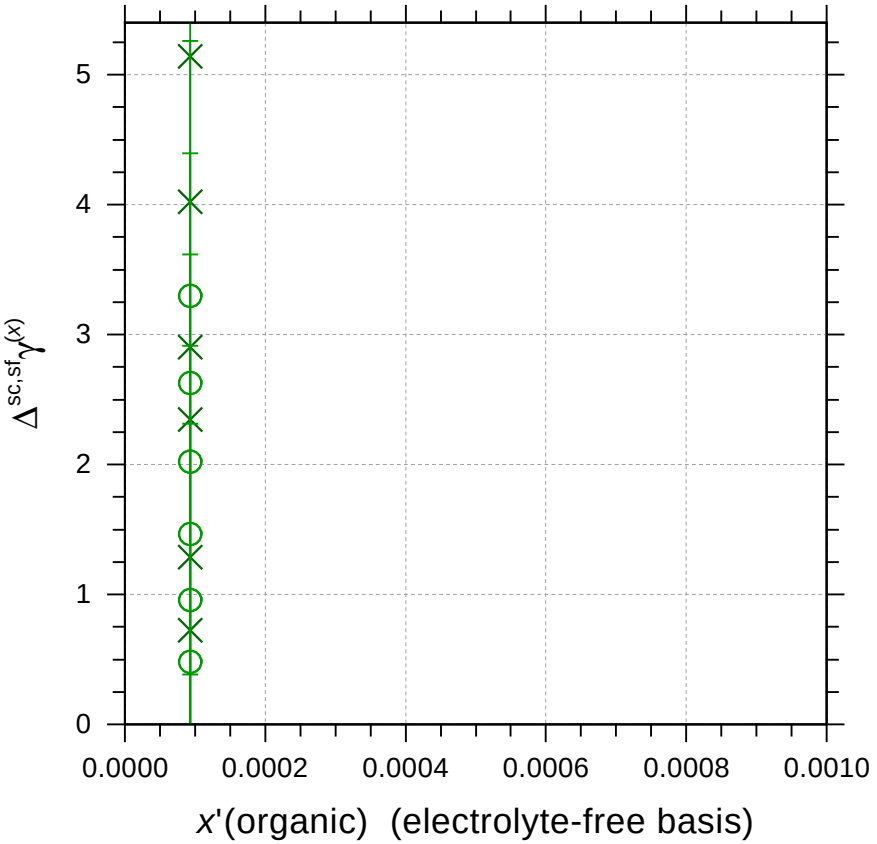


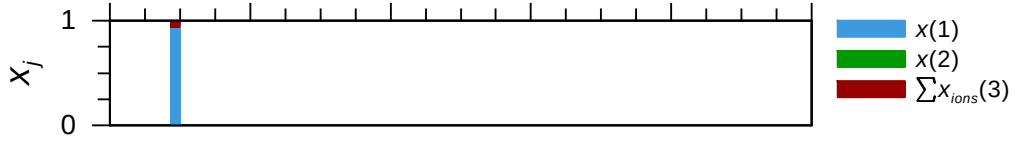
initial weighting of dataset:
$w^{init}(0110)$ = 1.000
dataset contribution to F_{obj}:
fval(0110) = 3.0319E-01
rel. contribution = 0.1442 %

Fig. S0114 (AIOMFAC_output_0979)

H_2O (1) + Ethanol (2) + Na_2SO_4 (3)

Temperature: 313 K



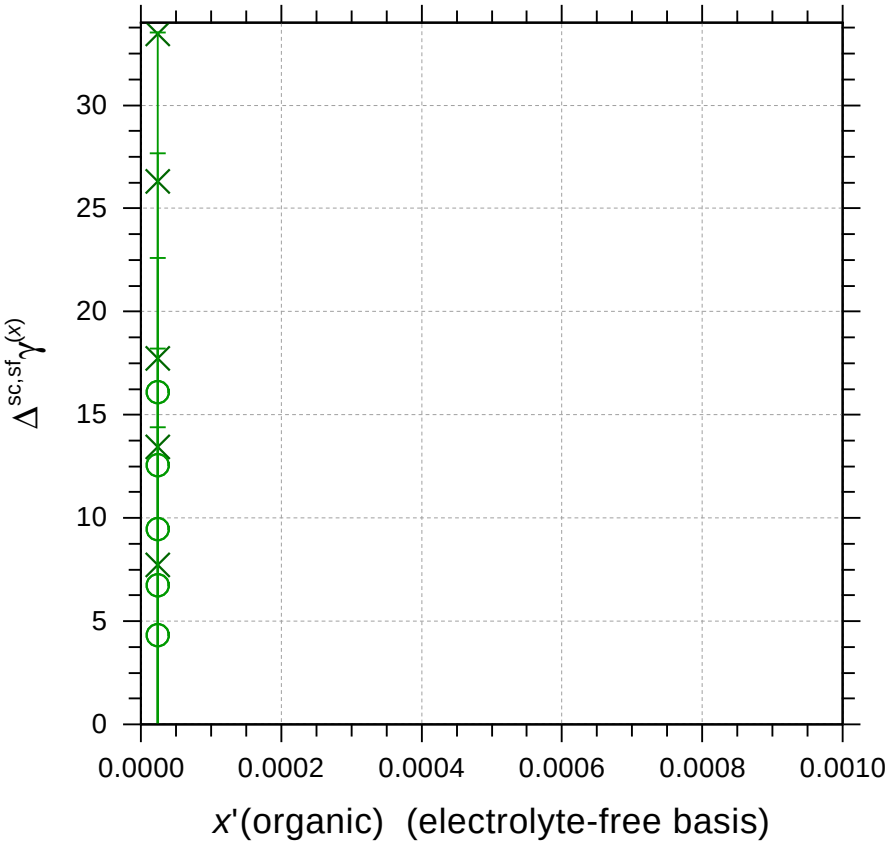


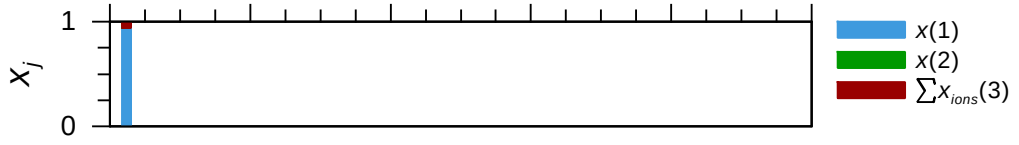
initial weighting of dataset:
w^{init}(0979) = 0.100
dataset contribution to F_{obj}:
fval(0979) = 1.3096E-02
rel. contribution = 0.0062 %

Fig. S0115 (AIOMFAC_output_0980)

H_2O (1) + 1-Propanol (2) + Na_2SO_4 (3)

Temperature: 313 K



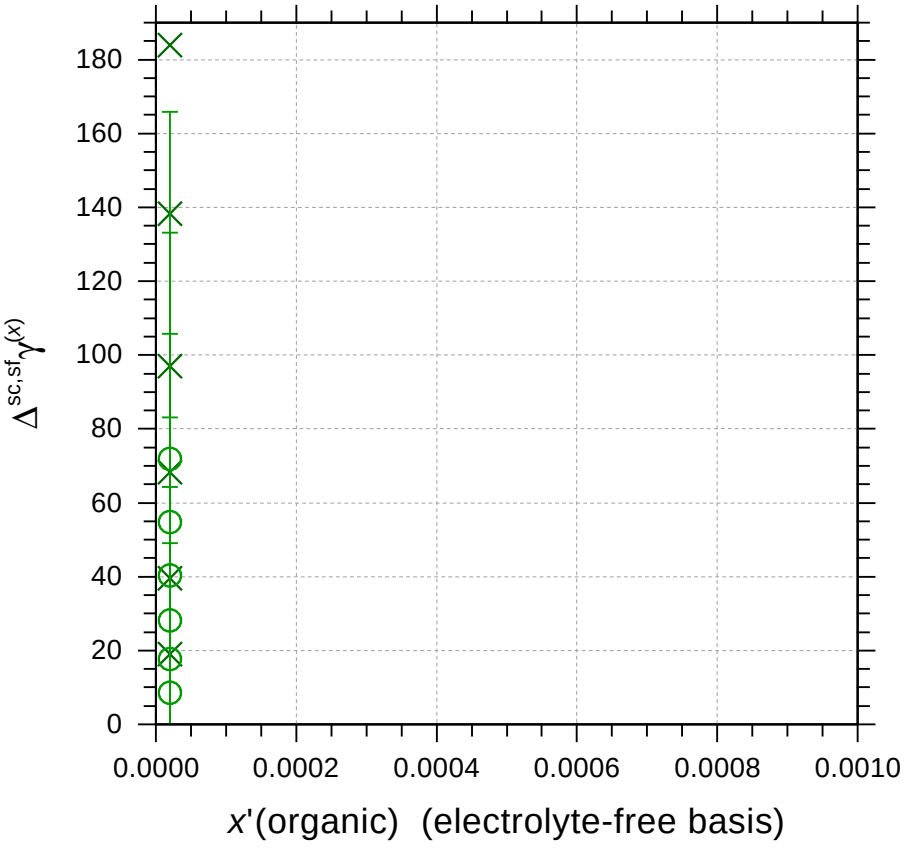


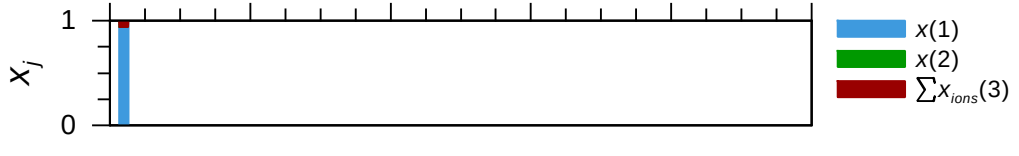
initial weighting of dataset:
w^{init}(0980) = 0.100
dataset contribution to F_{obj}:
fval(0980) = 3.8349E-02
rel. contribution = 0.0182 %

Fig. S0116 (AIOMFAC_output_0981)

H_2O (1) + 1-Butanol (2) + Na_2SO_4 (3)

Temperature: 313 K



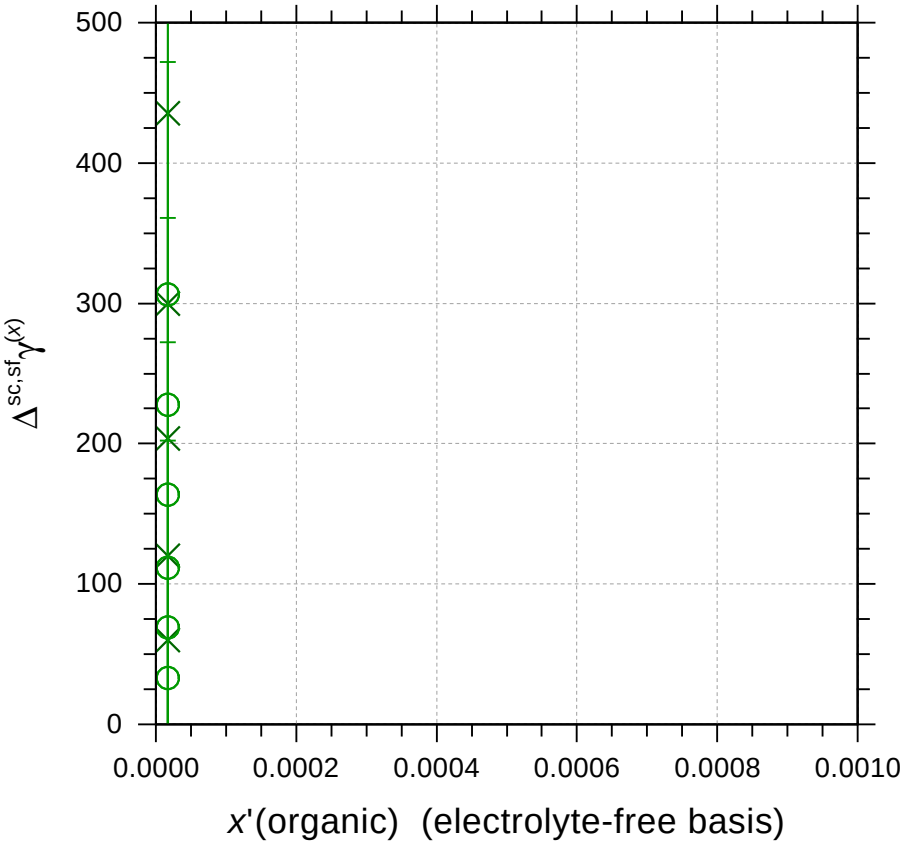


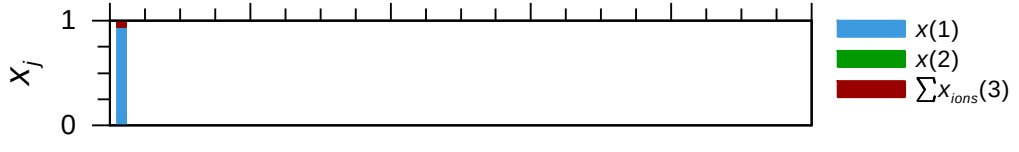
initial weighting of dataset:
$w^{init}(0981)$ = 0.100
dataset contribution to F_{obj}:
fval(0981) = 6.2505E-02
rel. contribution = 0.0297 %

Fig. S0117 (AIOMFAC_output_0982)

H_2O (1) + 1-Pentanol (2) + Na_2SO_4 (3)

Temperature: 313 K





left y-axis:

× Na2SO4+1-Pentanol+Water_VLE_Falabella (EXP, org.)

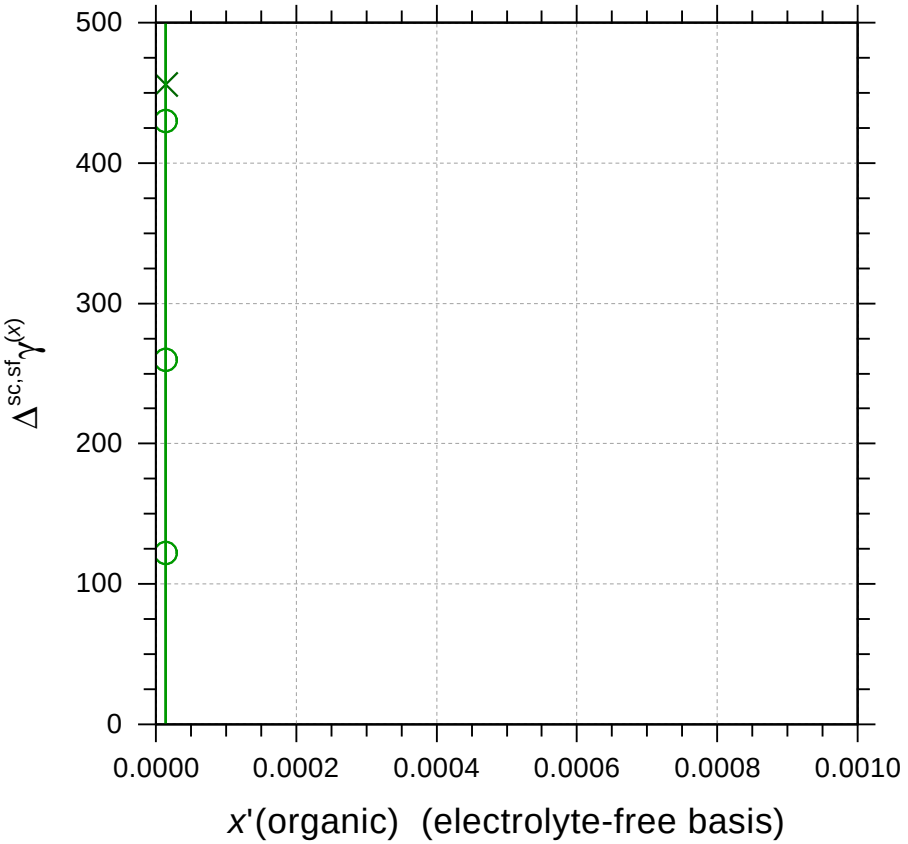
○ AIOMFAC $\Delta^{sc,sf}\gamma^{(x)}_{org.}$

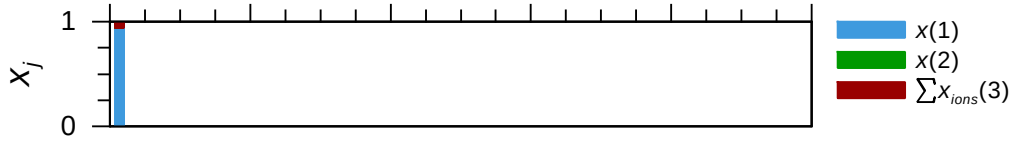
initial weighting of dataset:
$w^{init}(0982)$ = 0.100
dataset contribution to F_{obj}:
fval(0982) = 2.6336E-02
rel. contribution = 0.0125 %

Fig. S0118 (AIOMFAC_output_0983)

H_2O (1) + 1-Hexanol (2) + Na_2SO_4 (3)

Temperature: 313 K





left y-axis:

× Na2SO4+1-Hexanol+Water_VLE_Falabella (EXP, org.)

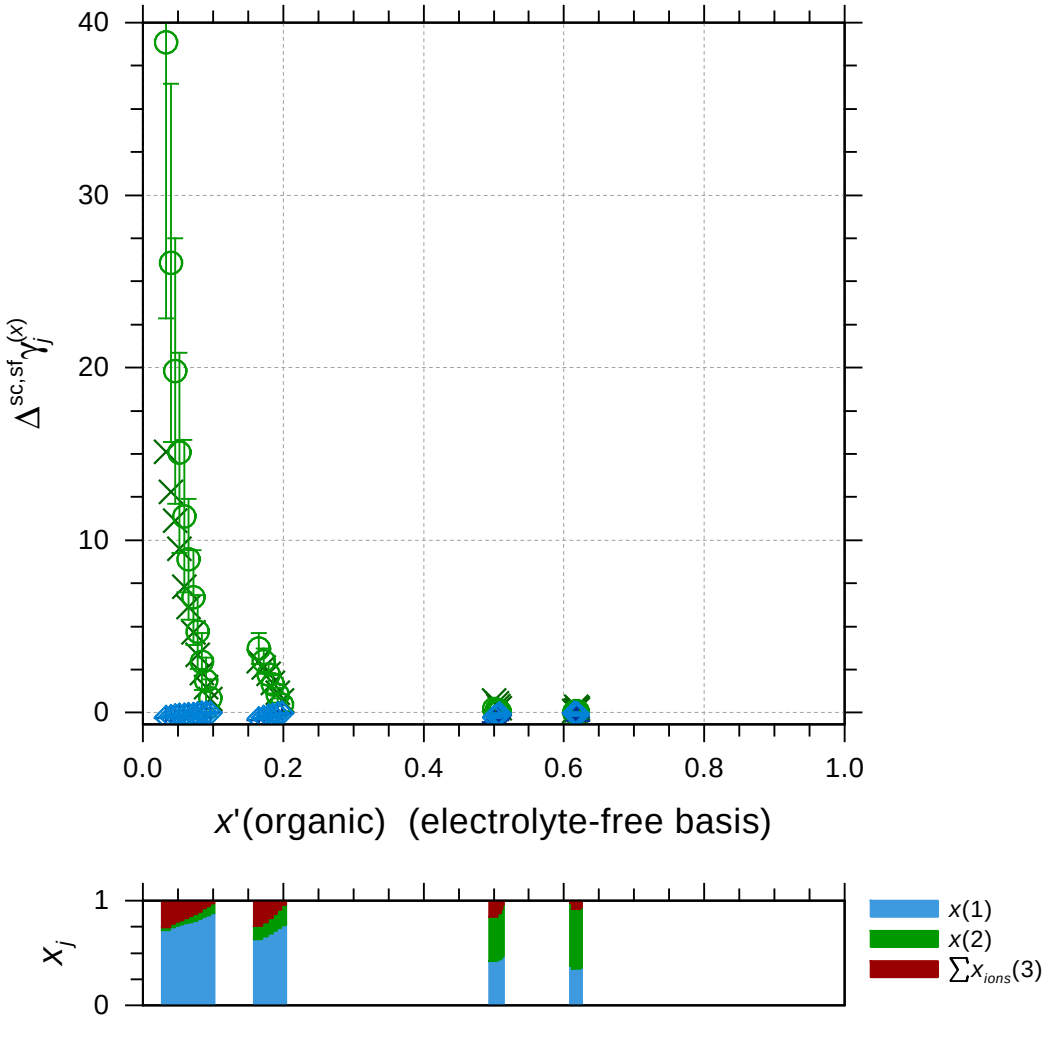
○ AIOMFAC $\Delta^{sc,sf}\gamma^{(x)}_{org.}$

initial weighting of dataset:
$w^{init}(0983)$ = 0.100
dataset contribution to F_{obj}:
fval(0983) = 9.9981E-02
rel. contribution = 0.0475 %

Fig. S0119 (AIOMFAC_output_0102)

H_2O (1) + 1-Propanol (2) + NaBr (3)

Temperature range: 360 -- 368 K

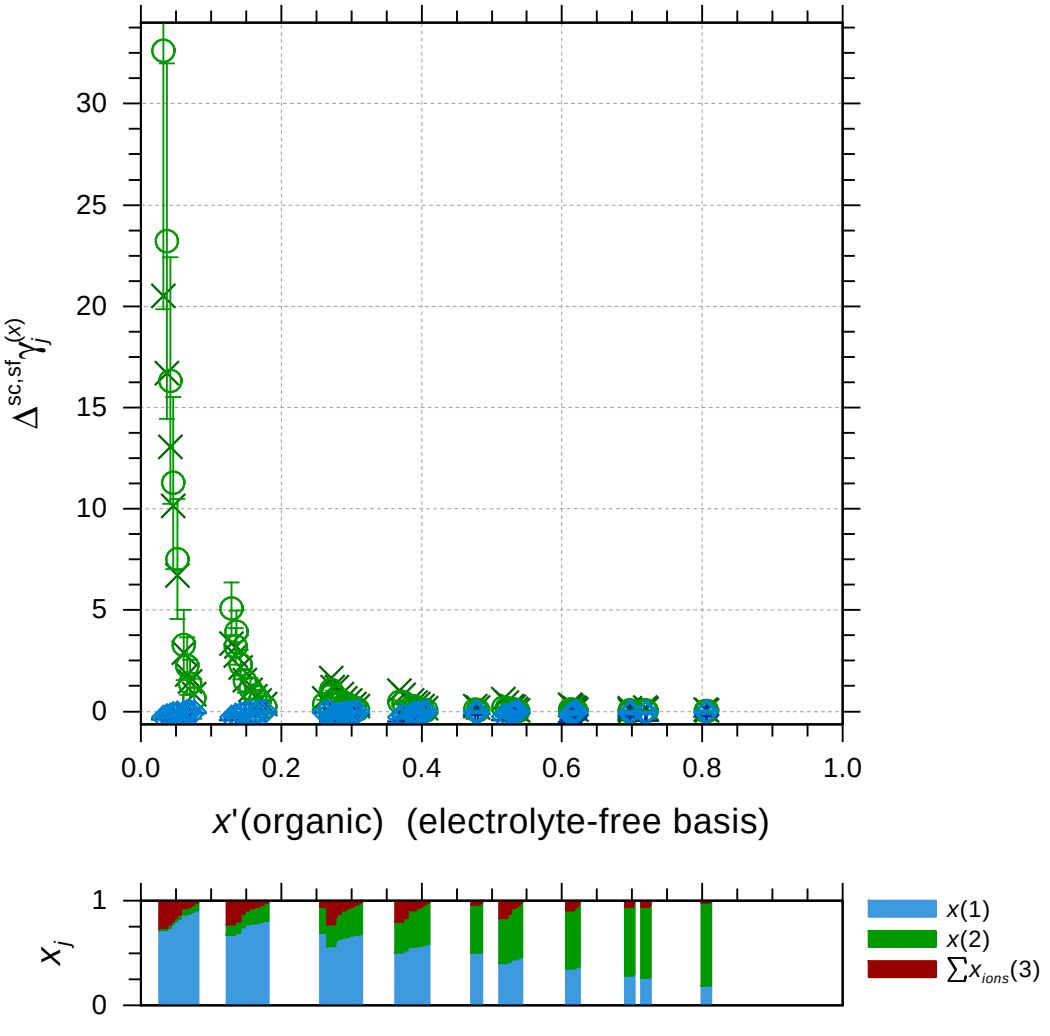


initial weighting of dataset:
$w^{init}(0102)$ = 0.500
dataset contribution to F_{obj}:
fval(0102) = 3.9347E-01
rel. contribution = 0.1871 %

Fig. S0120 (AIOMFAC_output_0103)

H_2O (1) + 2-Propanol (2) + NaBr (3)

Temperature range: 353 -- 358 K

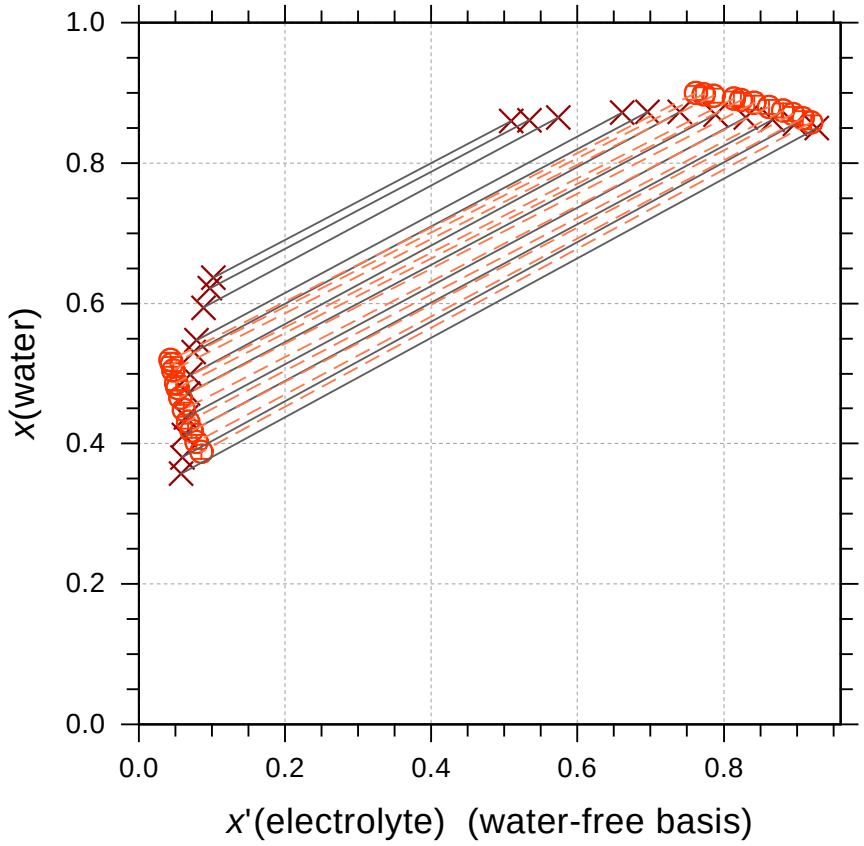


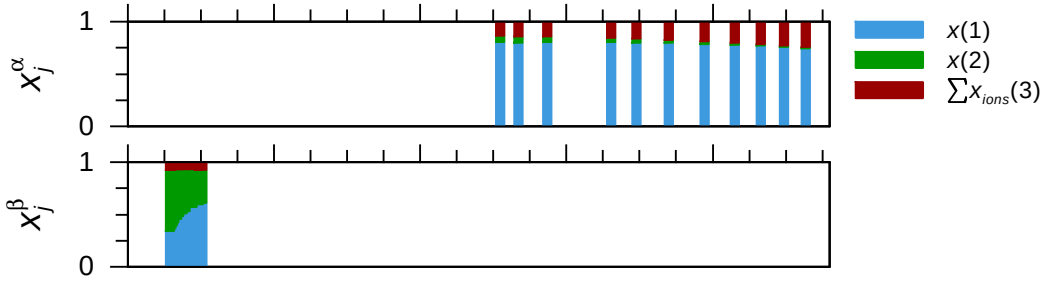
initial weighting of dataset:
$w^{init}(0103)$ = 0.500
dataset contribution to F_{obj}:
fval(0103) = 1.6713E-01
rel. contribution = 0.0795 %

Fig. S0121 (AIOMFAC_output_0104)

H_2O (1) + 1-Propanol (2) + NaBr (3)

Temperature: 298 K





left y-axis:

× NaBr_1-PrOH_LLE_Chou

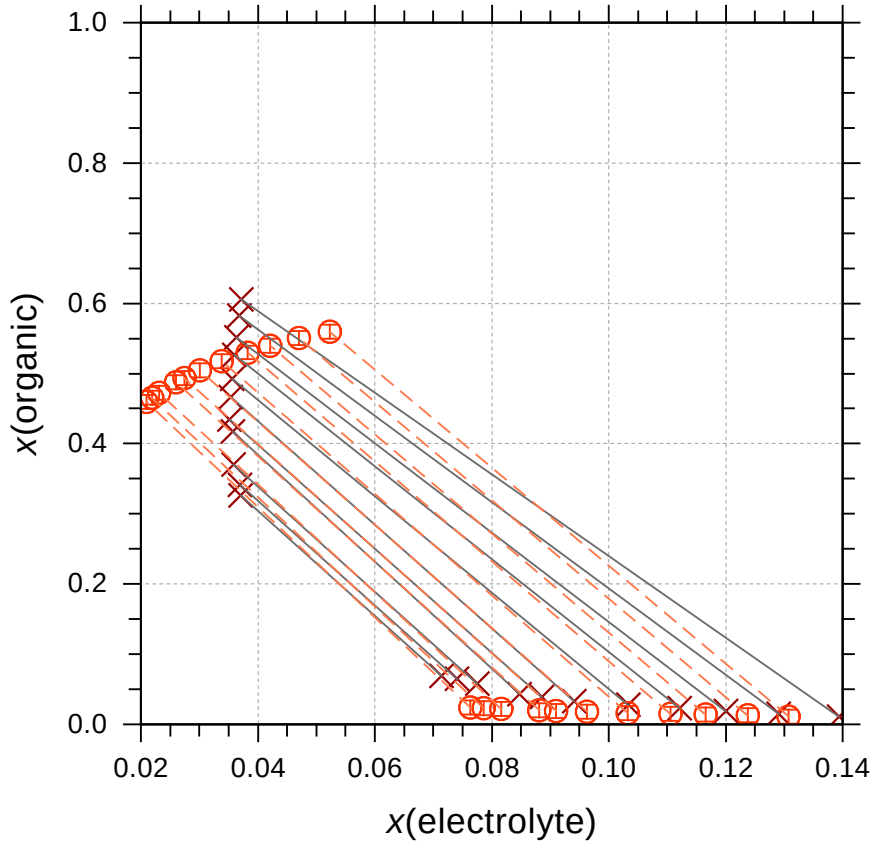
○ AIOMFAC calc. LLE composition

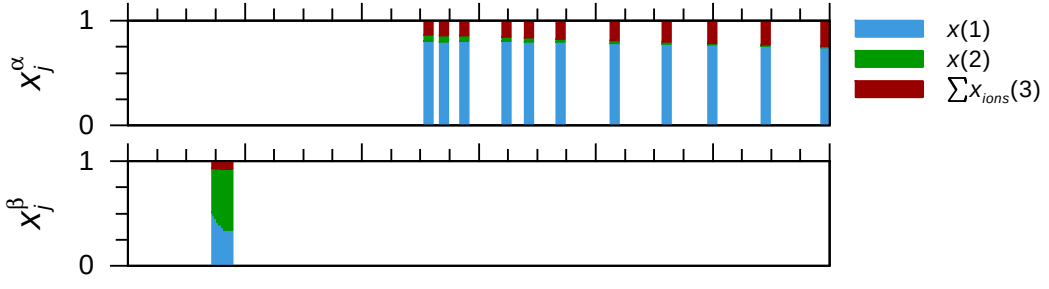
initial weighting of dataset:
w^{init}(0104) = 0.500
dataset contribution to F_{obj}:
fval(0104) = 2.2779E-01
rel. contribution = 0.1083 %

Fig. S0121a (AIOMFAC_output_0104)

H_2O (1) + 1-Propanol (2) + NaBr (3)

Temperature: 298 K



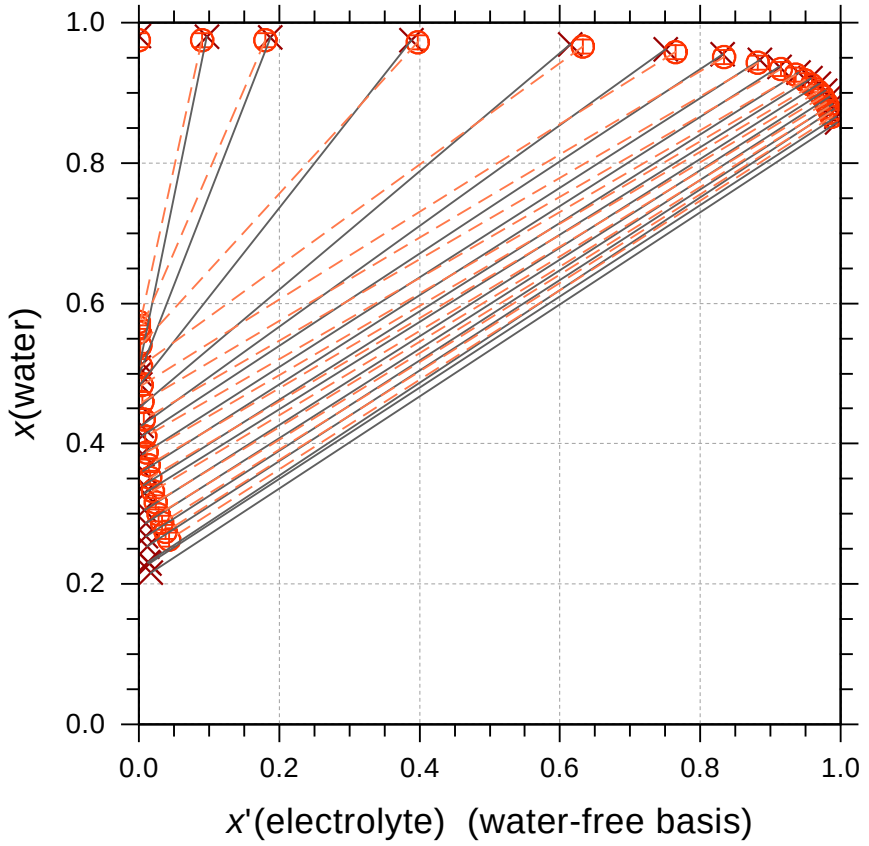


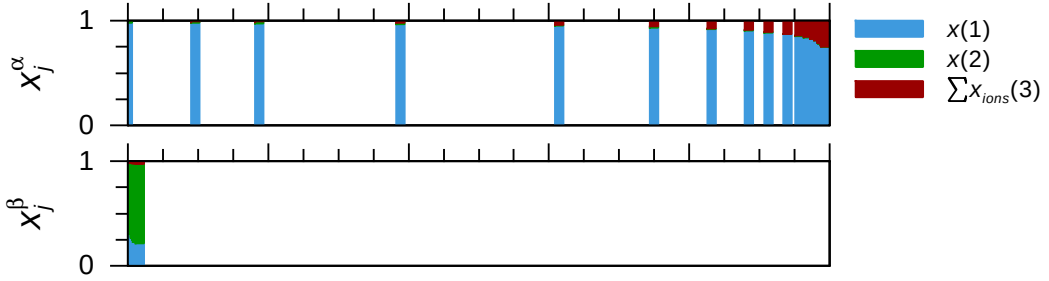
initial weighting of dataset:
$w^{init}(0104)$ = 0.500
dataset contribution to F_{obj}:
fval(0104) = 2.2779E-01
rel. contribution = 0.1083 %

Fig. S0122 (AIOMFAC_output_0975)

H_2O (1) + 1-Butanol (2) + NaBr (3)

Temperature: 298 K





left y-axis:

× NaBr+1-Butanol+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0975)$ = 1.000

dataset contribution to F_{obj}:

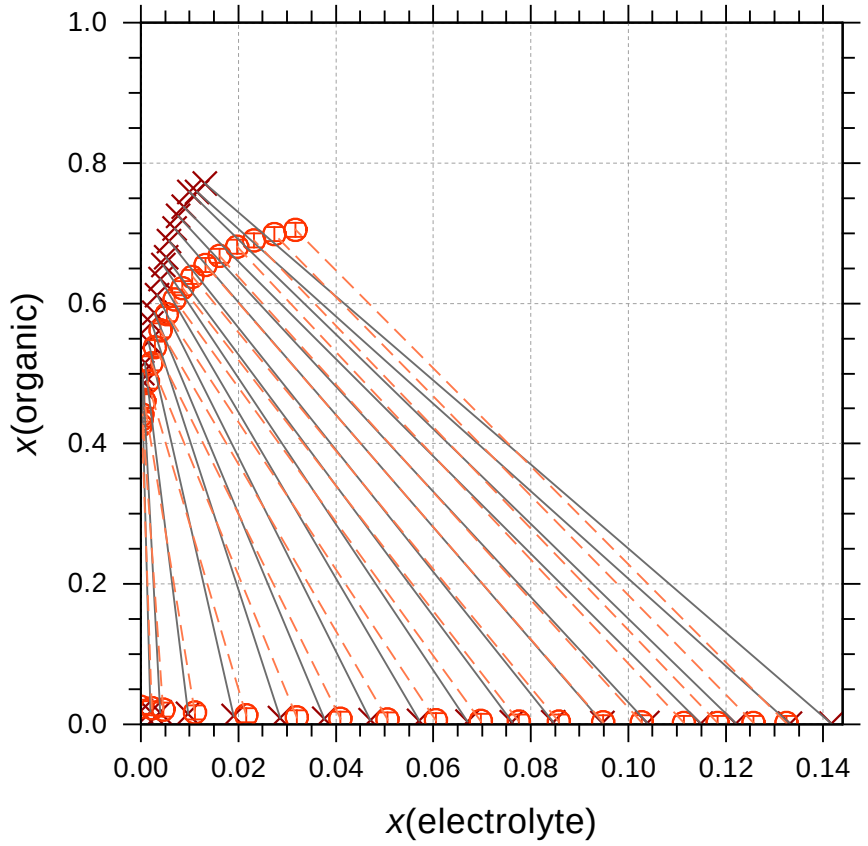
fval(0975) = 2.6418E-01

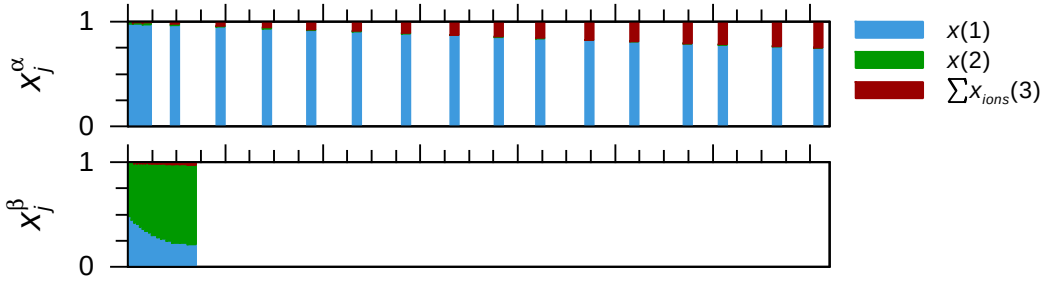
rel. contribution = 0.1256 %

Fig. S0122a (AIOMFAC_output_0975)

H_2O (1) + 1-Butanol (2) + NaBr (3)

Temperature: 298 K





left y-axis:

× NaBr+1-Butanol+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0975)$ = 1.000

dataset contribution to F_{obj}:

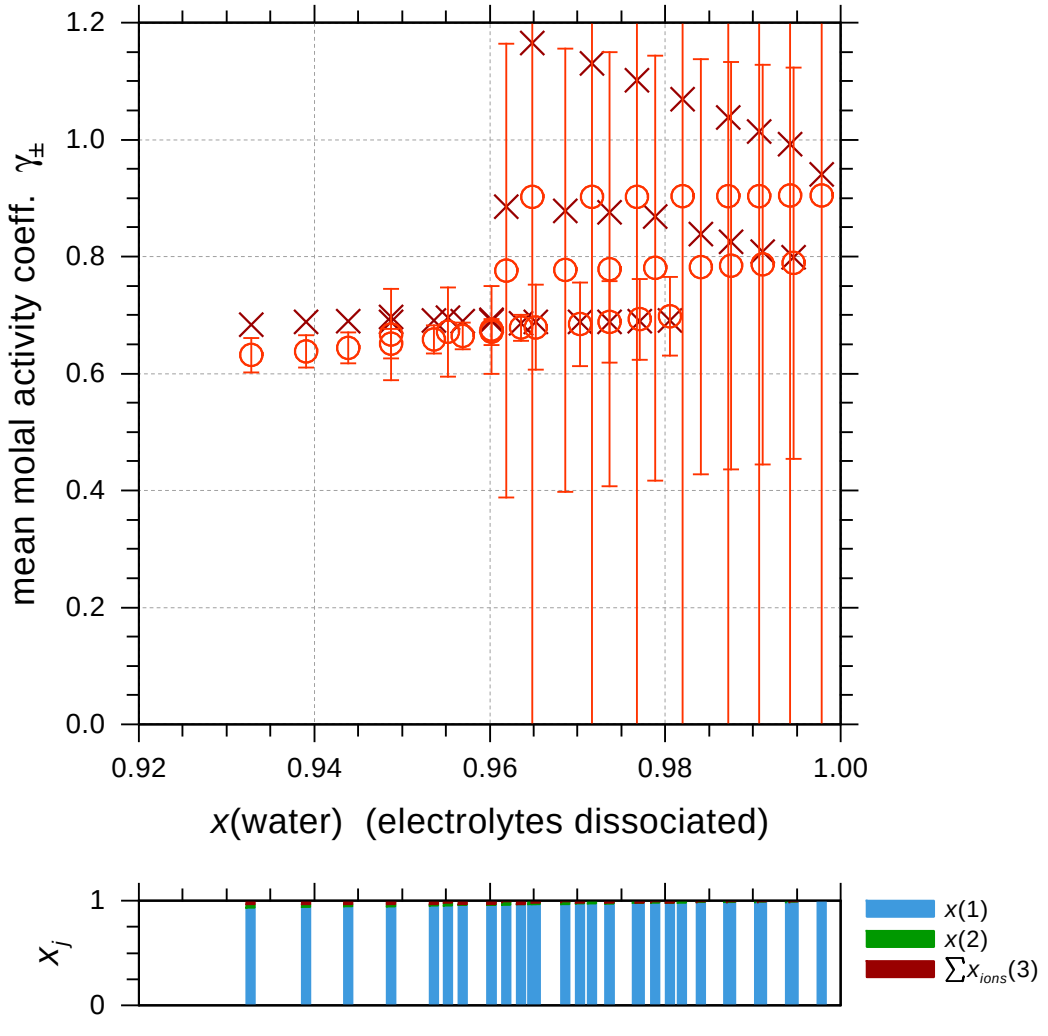
fval(0975) = 2.6418E-01

rel. contribution = 0.1256 %

Fig. S0123 (AIOMFAC_output_1042)

H_2O (1) + D-Mannopyranose (2) + NaBr (3)

Temperature: 298 K

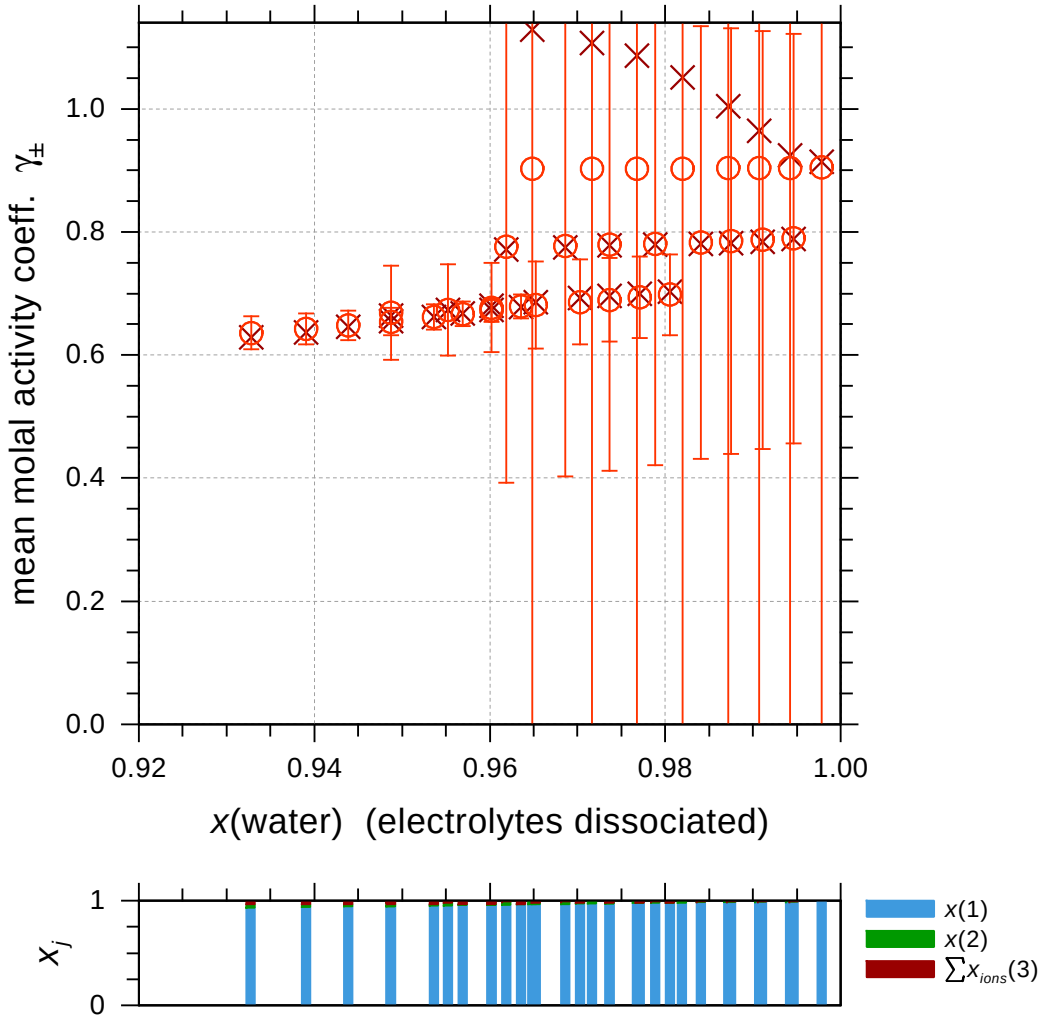


initial weighting of dataset:
$w^{init}(1042)$ = 2.000
dataset contribution to F_{obj}:
fval(1042) = 4.5787E-02
rel. contribution = 0.0218 %

Fig. S0124 (AIOMFAC_output_1045)

H_2O (1) + D-Ribofuranose (2) + NaBr (3)

Temperature: 298 K

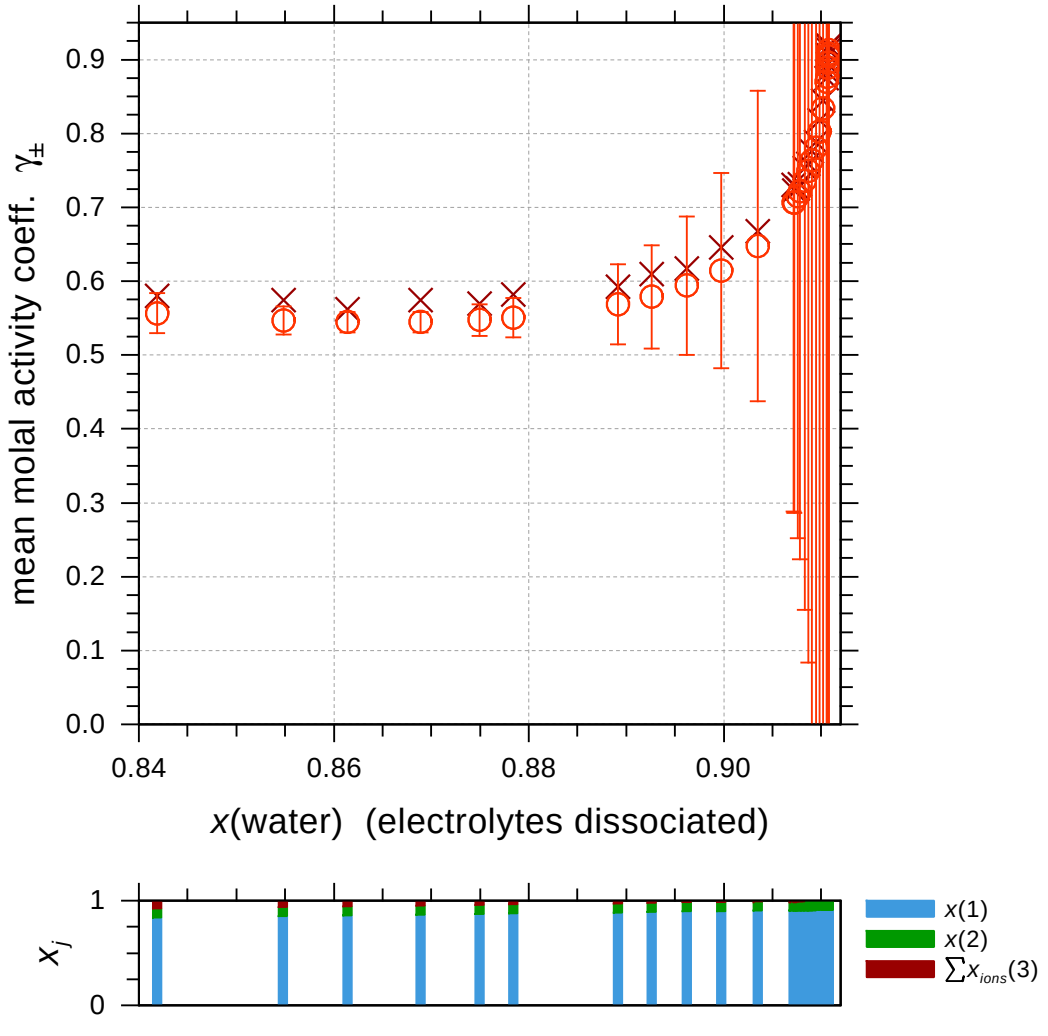


initial weighting of dataset:
$w^{init}(1045)$ = 2.000
dataset contribution to F_{obj}:
fval(1045) = 9.2774E-03
rel. contribution = 0.0044 %

Fig. S0125 (AIOMFAC_output_0008)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K

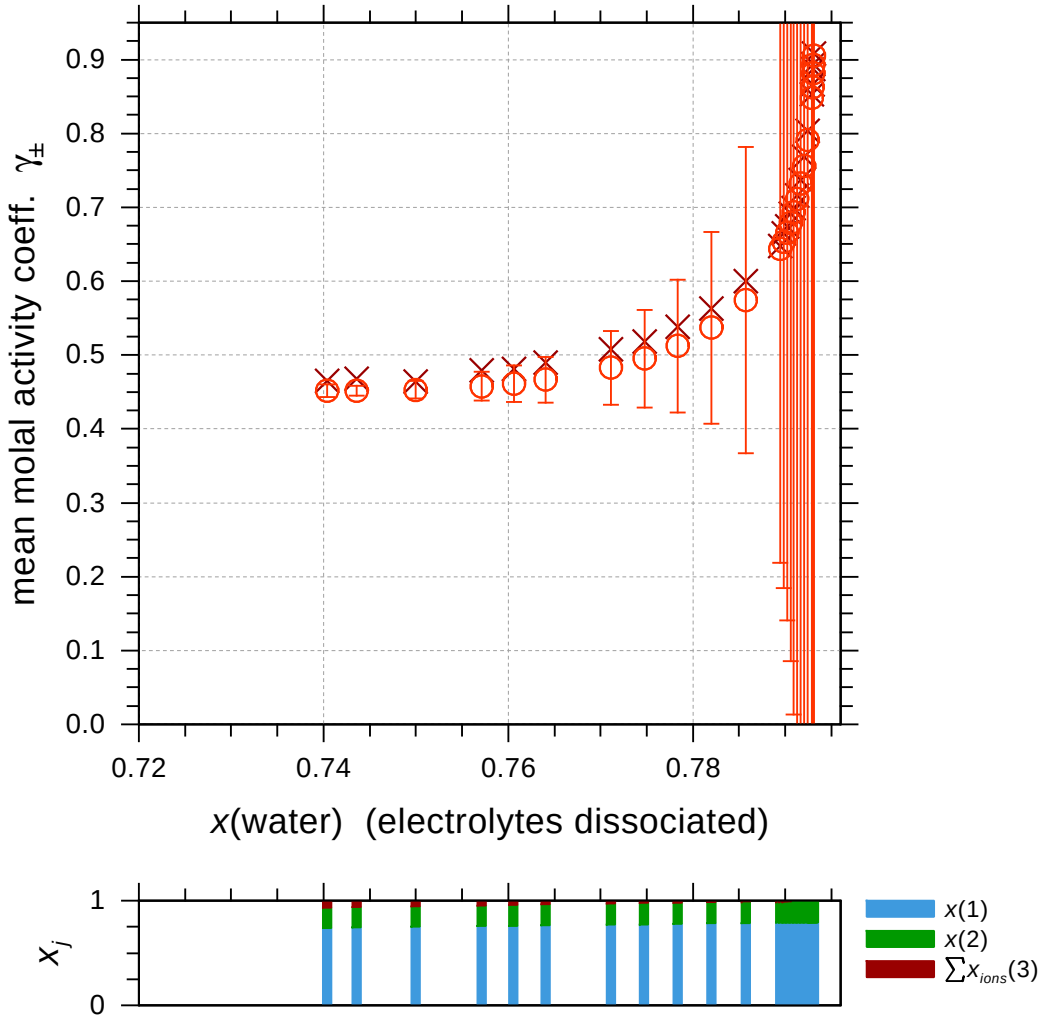


initial weighting of dataset:
w^{init}(0008) = 2.000
dataset contribution to F_{obj}:
fval(0008) = 1.3458E-02
rel. contribution = 0.0064 %

Fig. S0126 (AIOMFAC_output_0009)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K

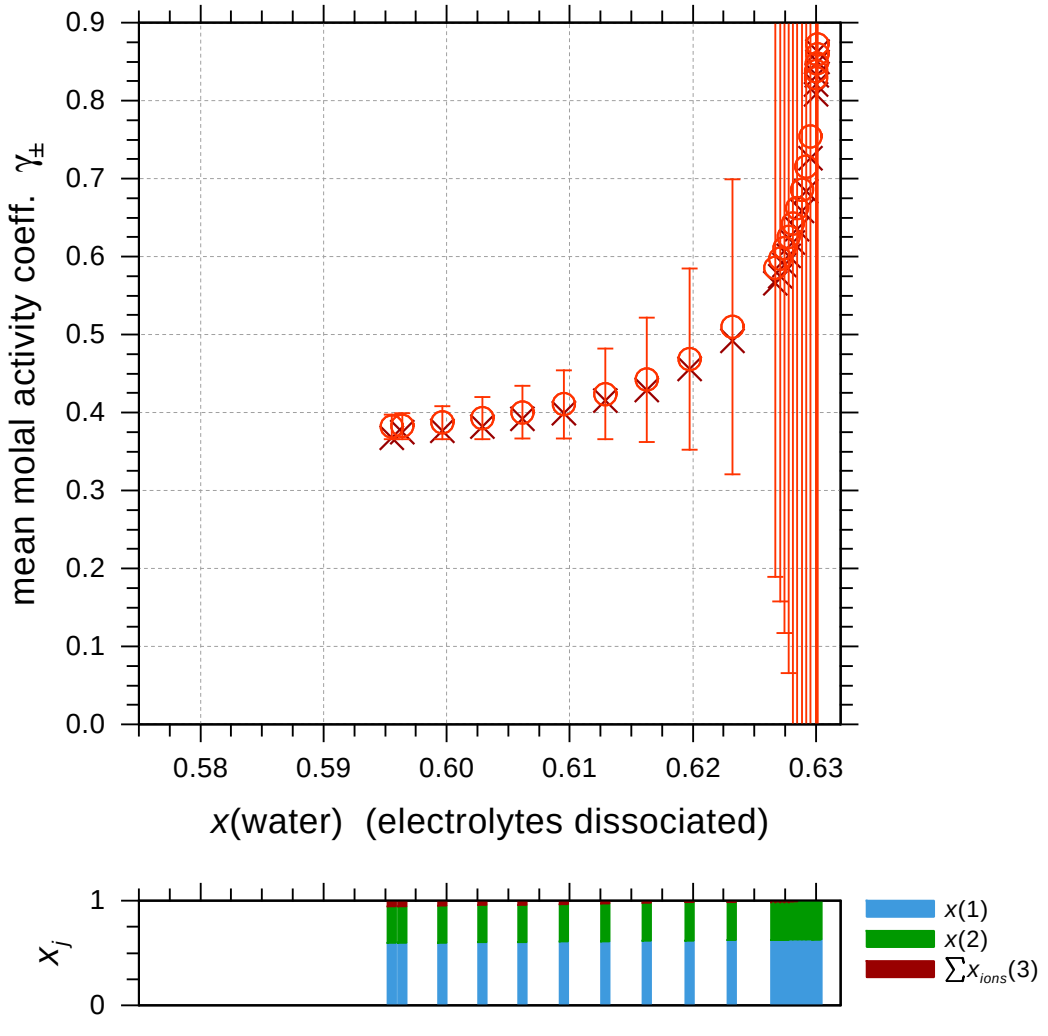


initial weighting of dataset:
$w^{init}(0009)$ = 2.000
dataset contribution to F_{obj}:
fval(0009) = 1.2633E-02
rel. contribution = 0.0060 %

Fig. S0127 (AIOMFAC_output_0010)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K

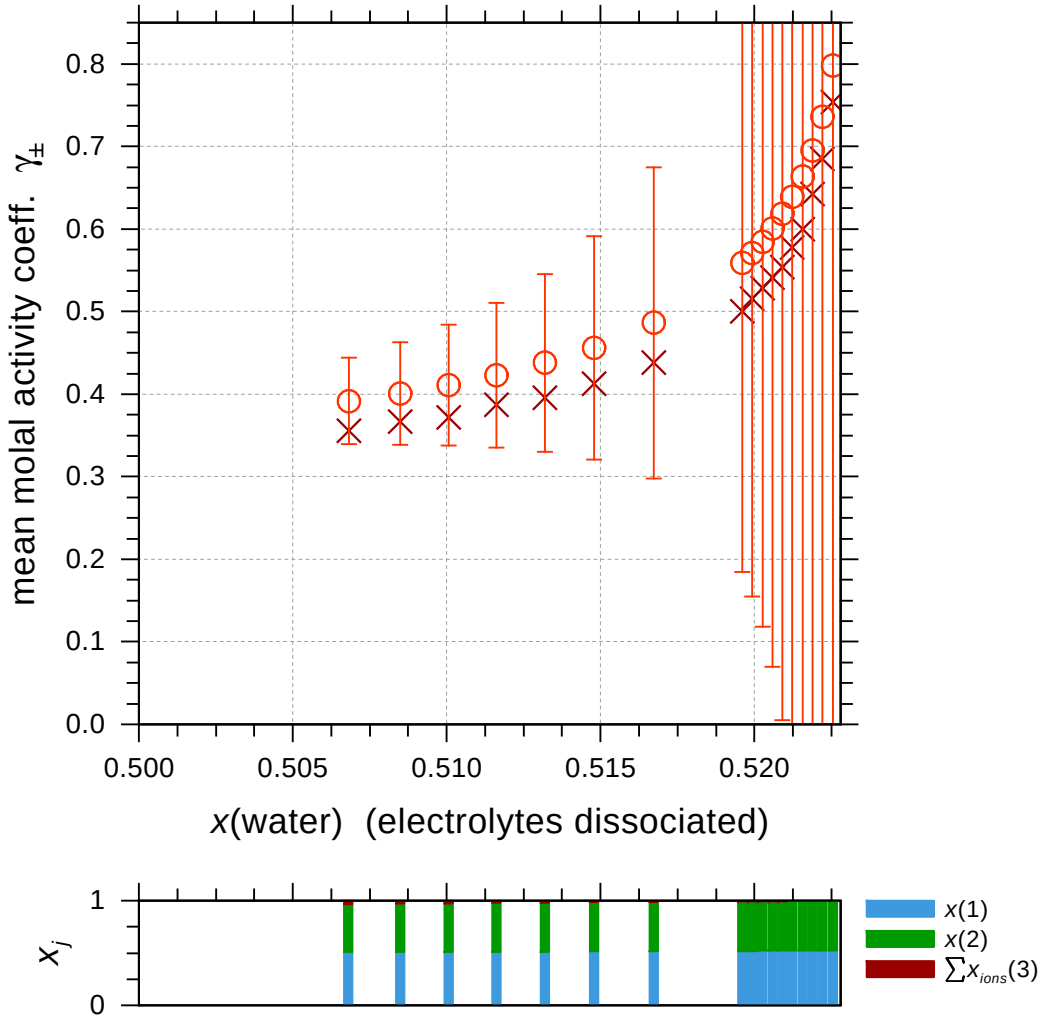


initial weighting of dataset:
$w^{init}(0010)$ = 2.000
dataset contribution to F_{obj}:
fval(0010) = 7.8957E-03
rel. contribution = 0.0038 %

Fig. S0128 (AIOMFAC_output_0011)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K

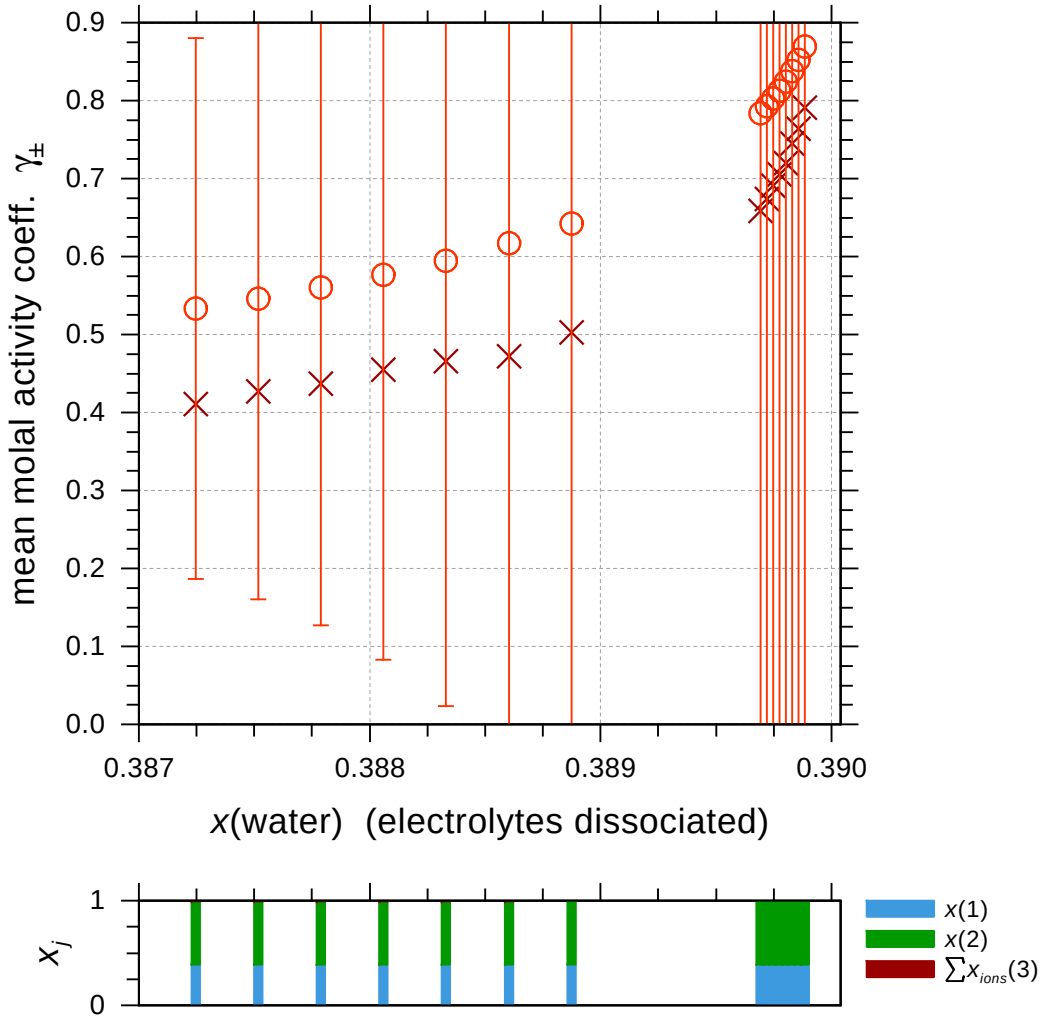


initial weighting of dataset:
$w^{init}(0011)$ = 1.000
dataset contribution to F_{obj}:
fval(0011) = 4.0843E-02
rel. contribution = 0.0194 %

Fig. S0129 (AIOMFAC_output_0012)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K

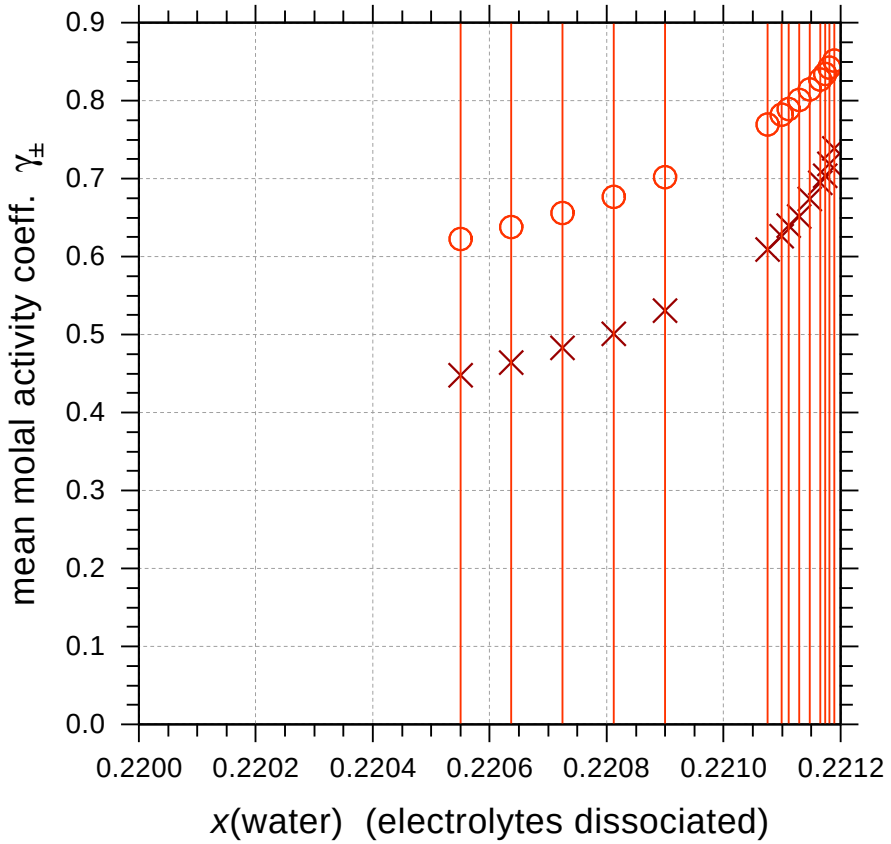


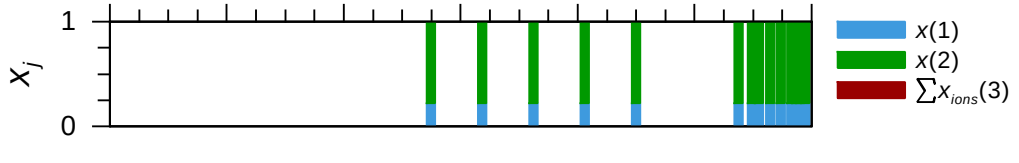
initial weighting of dataset:
$w^{init}(0012)$ = 0.500
dataset contribution to F_{obj}:
fval(0012) = 4.4192E-02
rel. contribution = 0.0210 %

Fig. S0130 (AIOMFAC_output_0013)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K



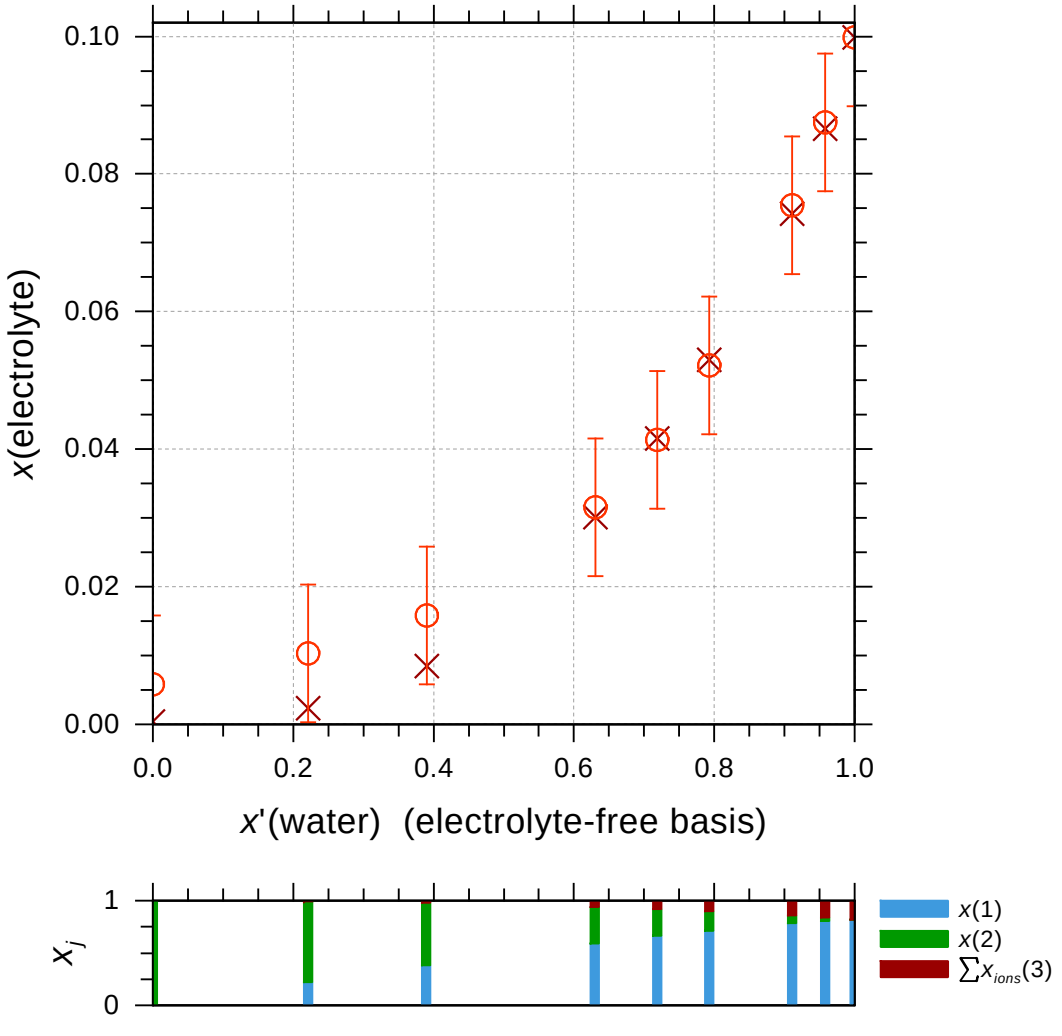


initial weighting of dataset:
$w^{init}(0013)$ = 0.500
dataset contribution to F_{obj}:
fval(0013) = 3.0701E-02
rel. contribution = 0.0146 %

Fig. S0131 (AIOMFAC_output_0016)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K

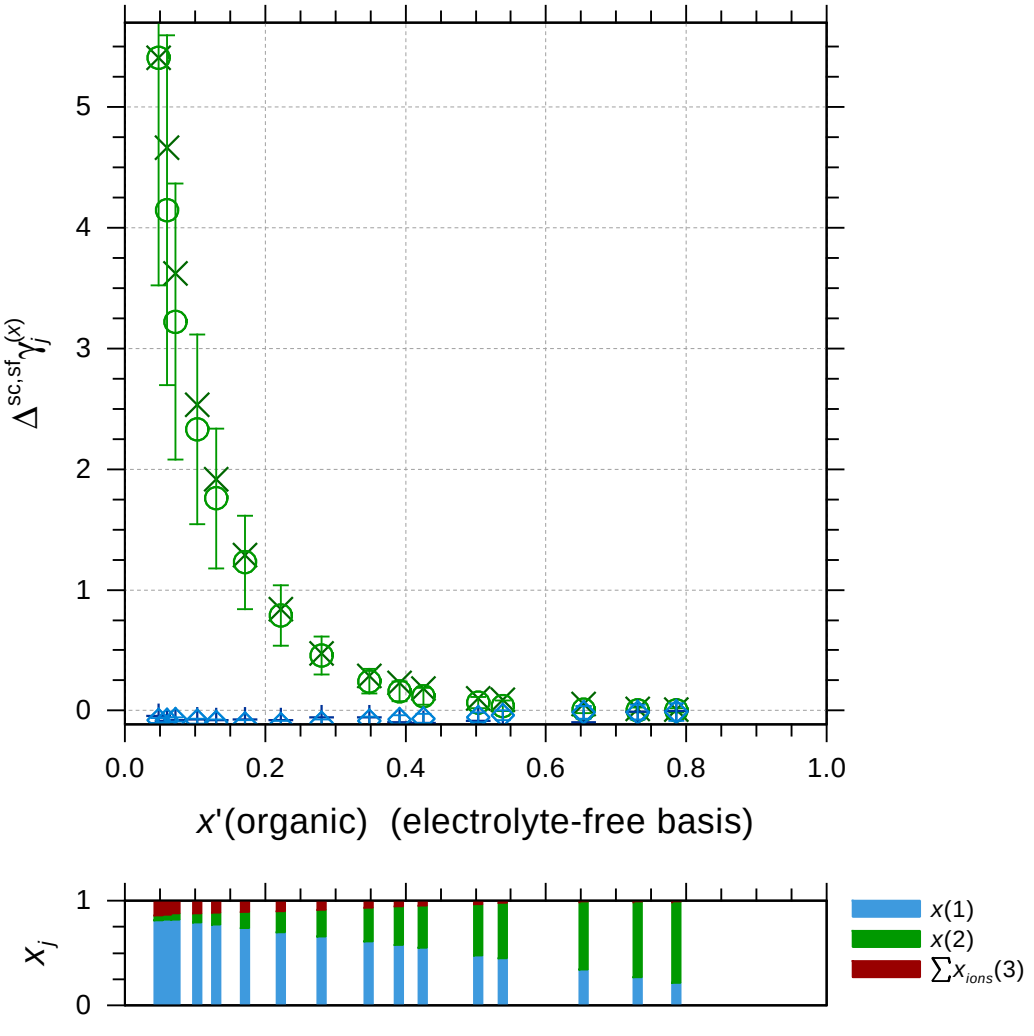


initial weighting of dataset:
$w^{init}(0016)$ = 1.000
dataset contribution to F_{obj}:
fval(0016) = 8.3974E-01
rel. contribution = 0.3993 %

Fig. S0132 (AIOMFAC_output_0017)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature range: 306 -- 313 K

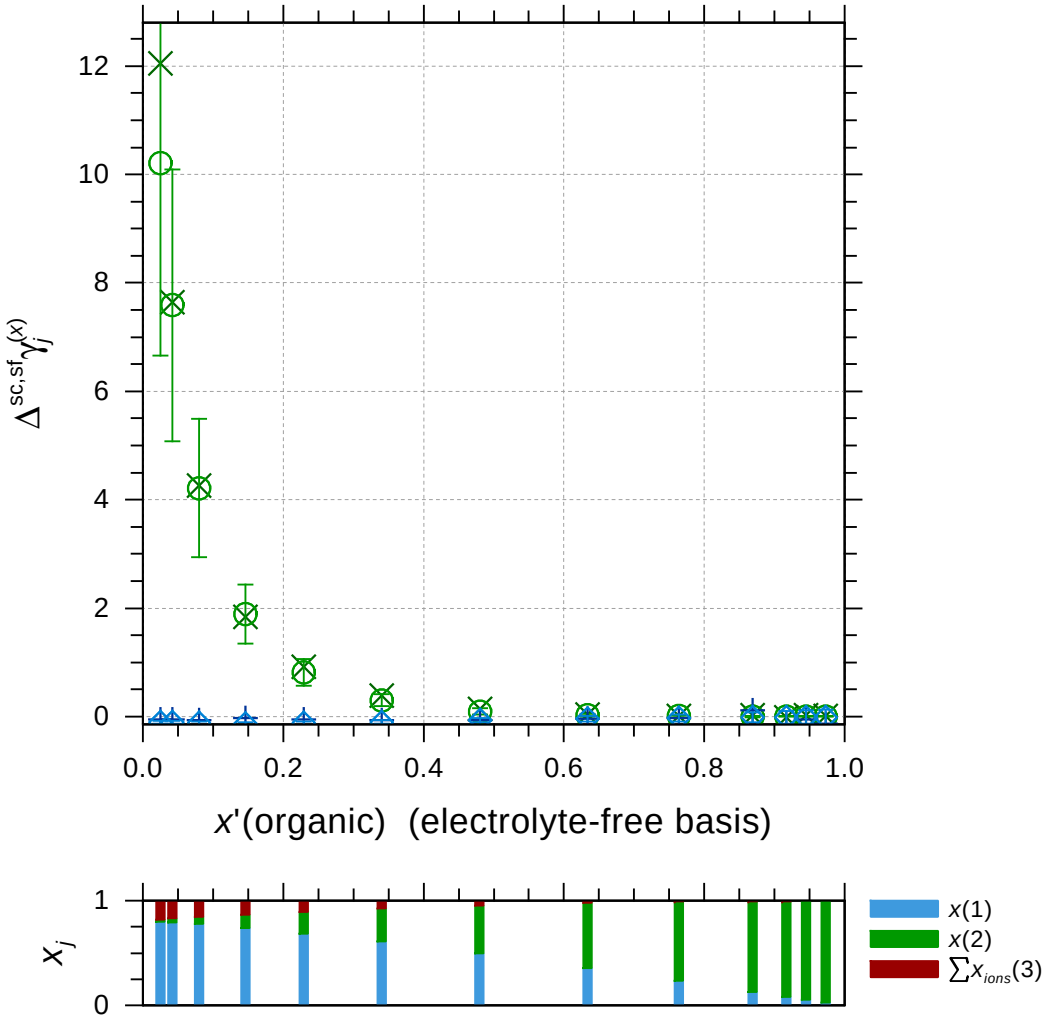


initial weighting of dataset:
$w^{init}(0017)$ = 0.500
dataset contribution to F_{obj}:
fval(0017) = 1.3699E-02
rel. contribution = 0.0065 %

Fig. S0133 (AIOMFAC_output_0018)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature range: 350 -- 362 K



initial weighting of dataset:

$w^{init}(0018)$ = 0.500

dataset contribution to F_{obj}:

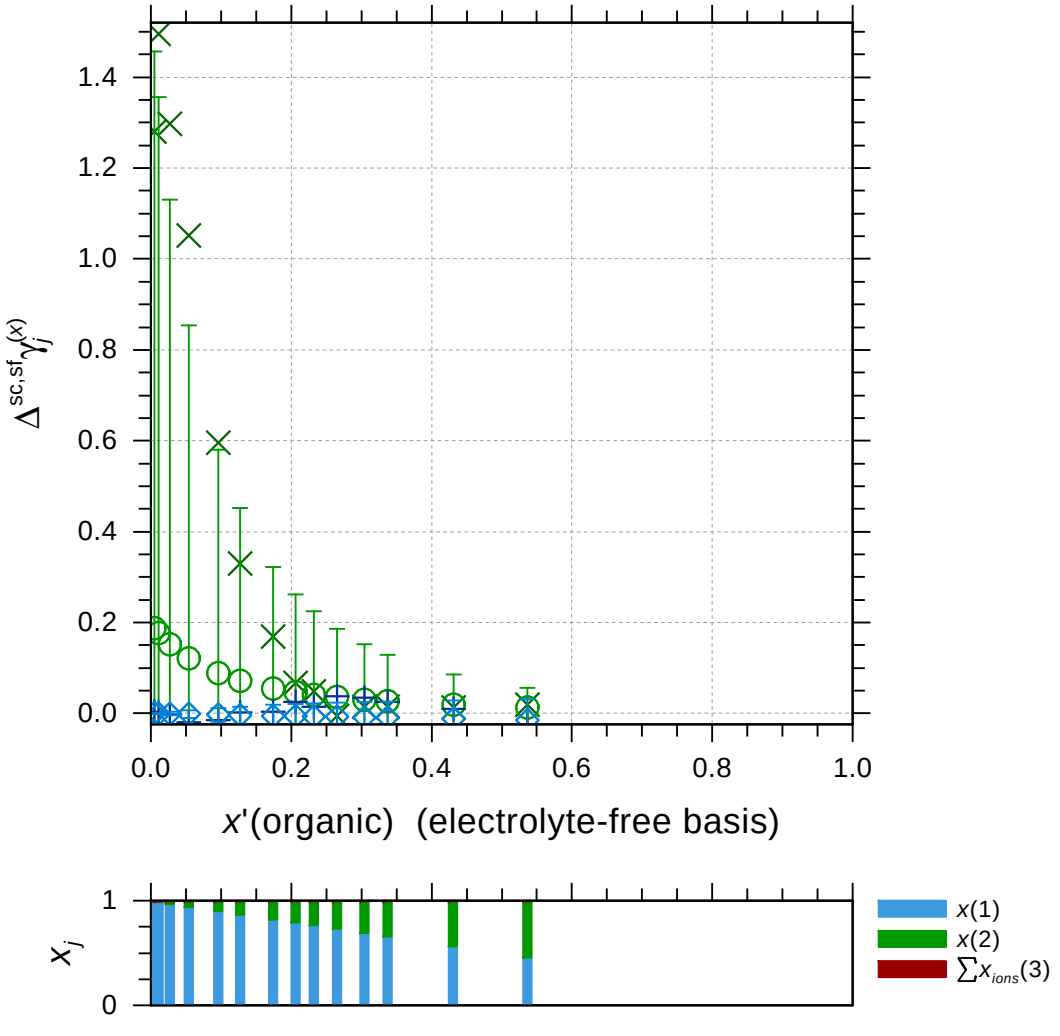
fval(0018) = 2.8045E-02

rel. contribution = 0.0133 %

Fig. S0134 (AIOMFAC_output_0019)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature range: 317 -- 332 K



initial weighting of dataset:

$w^{init}(0019)$ = 0.500

dataset contribution to F_{obj}:

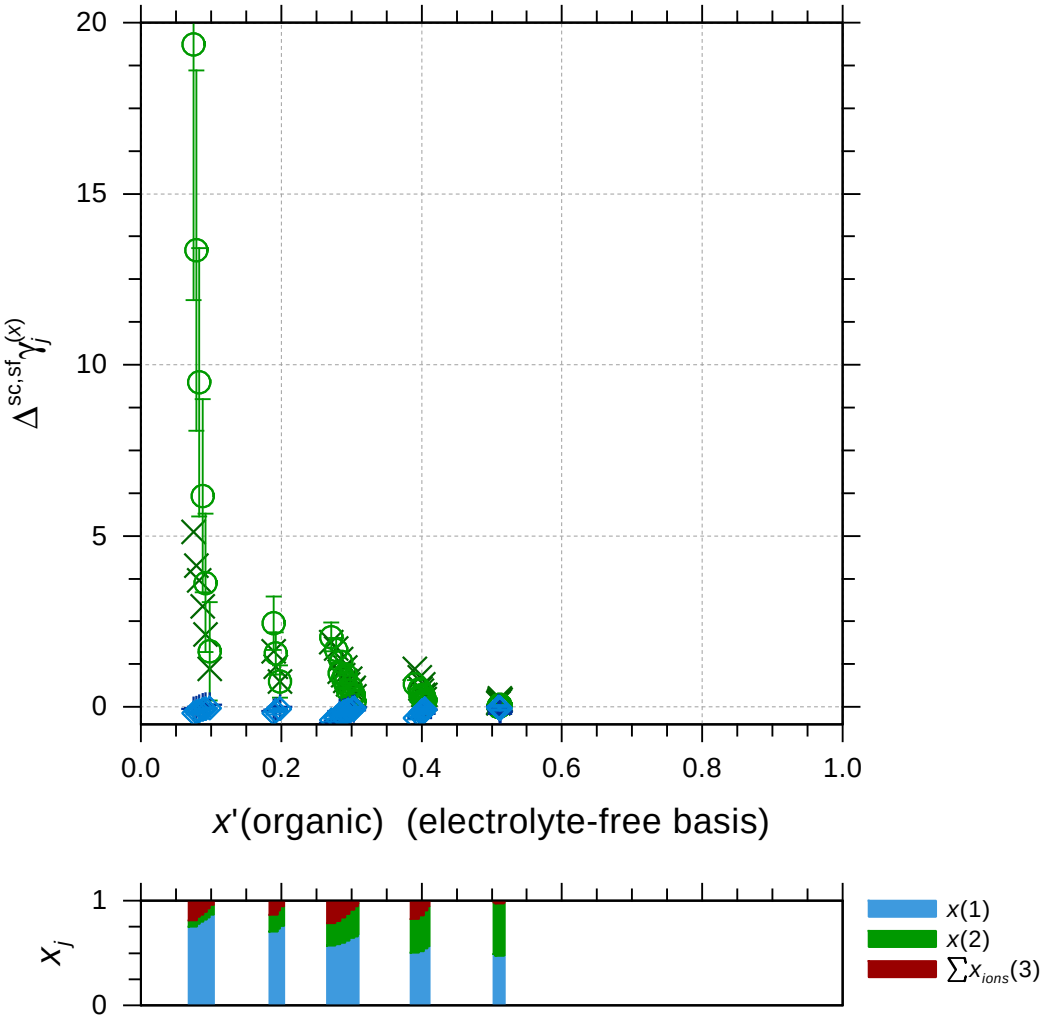
fval(0019) = 1.9793E-01

rel. contribution = 0.0941 %

Fig. S0135 (AIOMFAC_output_0020)

H_2O (1) + 1-Propanol (2) + NaCl (3)

Temperature range: 359 -- 364 K

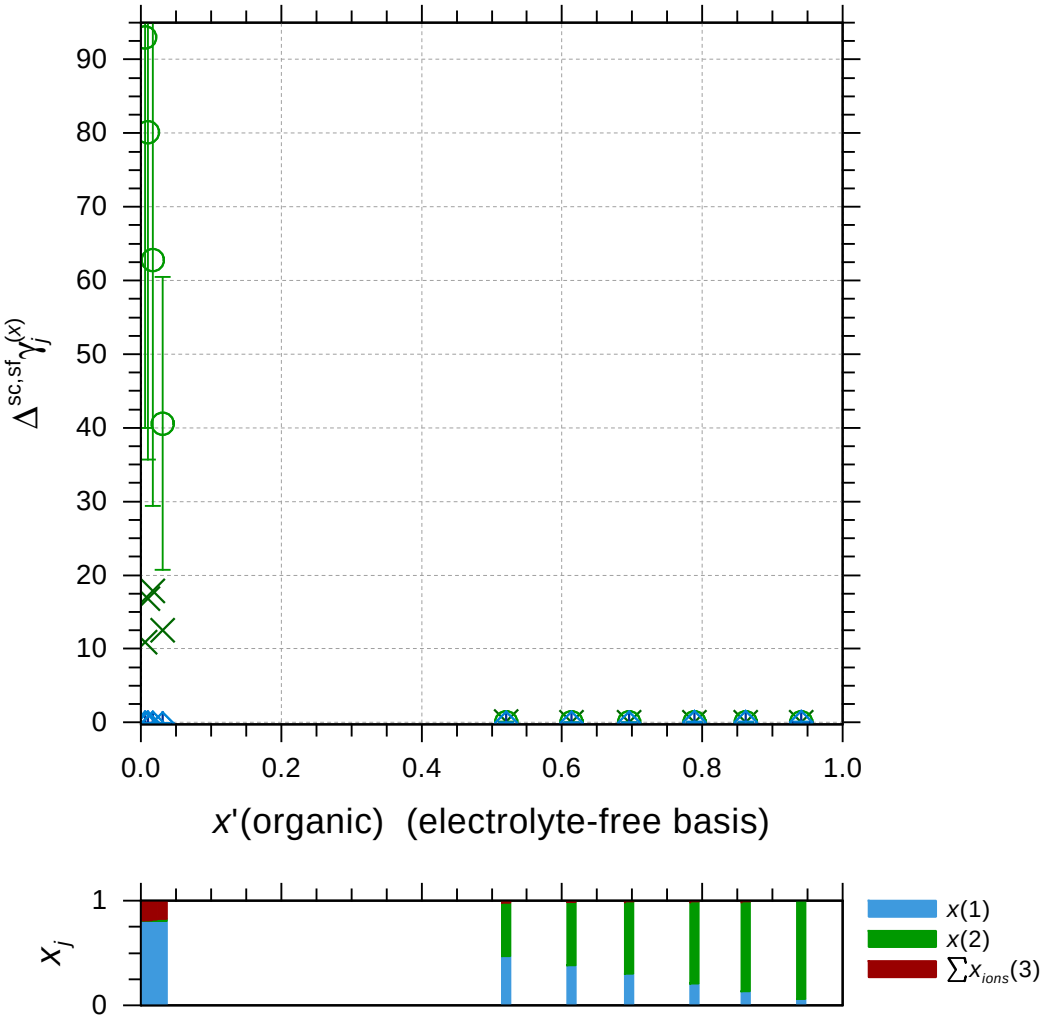


initial weighting of dataset:
$w^{init}(0020)$ = 0.500
dataset contribution to F_{obj}:
fval(0020) = 4.4964E-01
rel. contribution = 0.2138 %

Fig. S0136 (AIOMFAC_output_0021)

H_2O (1) + 1-Propanol (2) + NaCl (3)

Temperature range: 362 -- 376 K

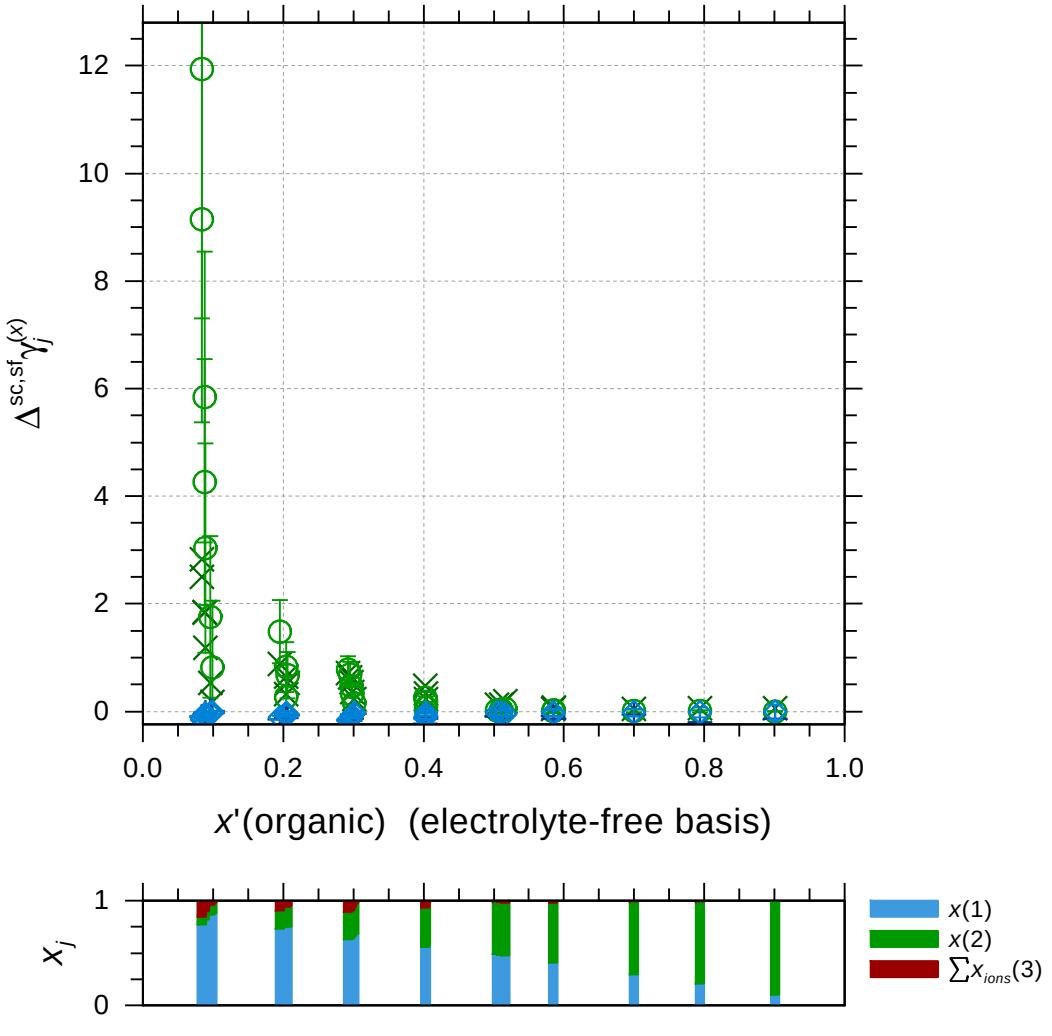


initial weighting of dataset:
$w^{init}(0021)$ = 0.500
dataset contribution to F_{obj}:
fval(0021) = 2.0918E+00
rel. contribution = 0.9947 %

Fig. S0137 (AIOMFAC_output_0022)

H_2O (1) + 1-Propanol (2) + NaCl (3)

Temperature range: 361 -- 366 K



initial weighting of dataset:

$w^{init}(0022)$ = 0.500

dataset contribution to F_{obj}:

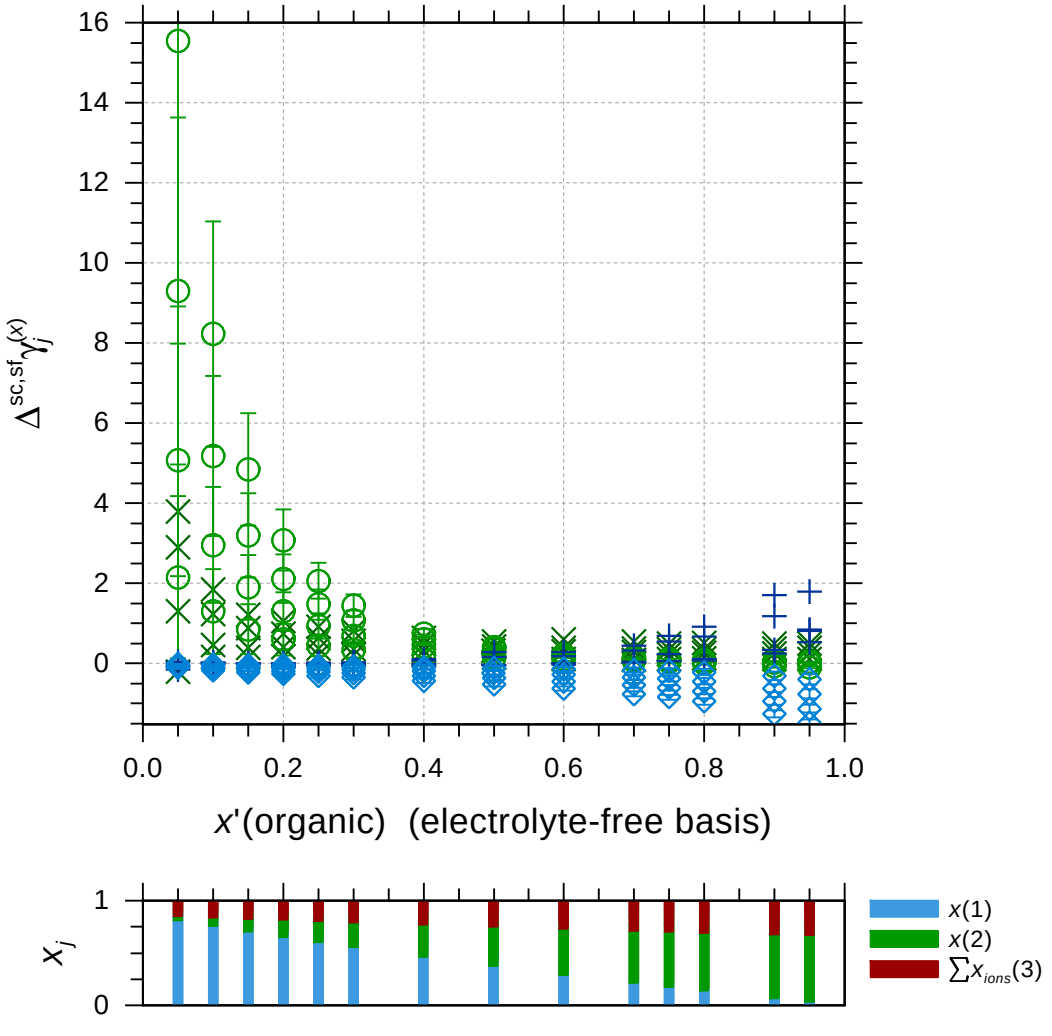
fval(0022) = 6.3689E-01

rel. contribution = 0.3029 %

Fig. S0138 (AIOMFAC_output_0023)

H_2O (1) + 2-Propanol (2) + NaCl (3)

Temperature range: 353 -- 362 K

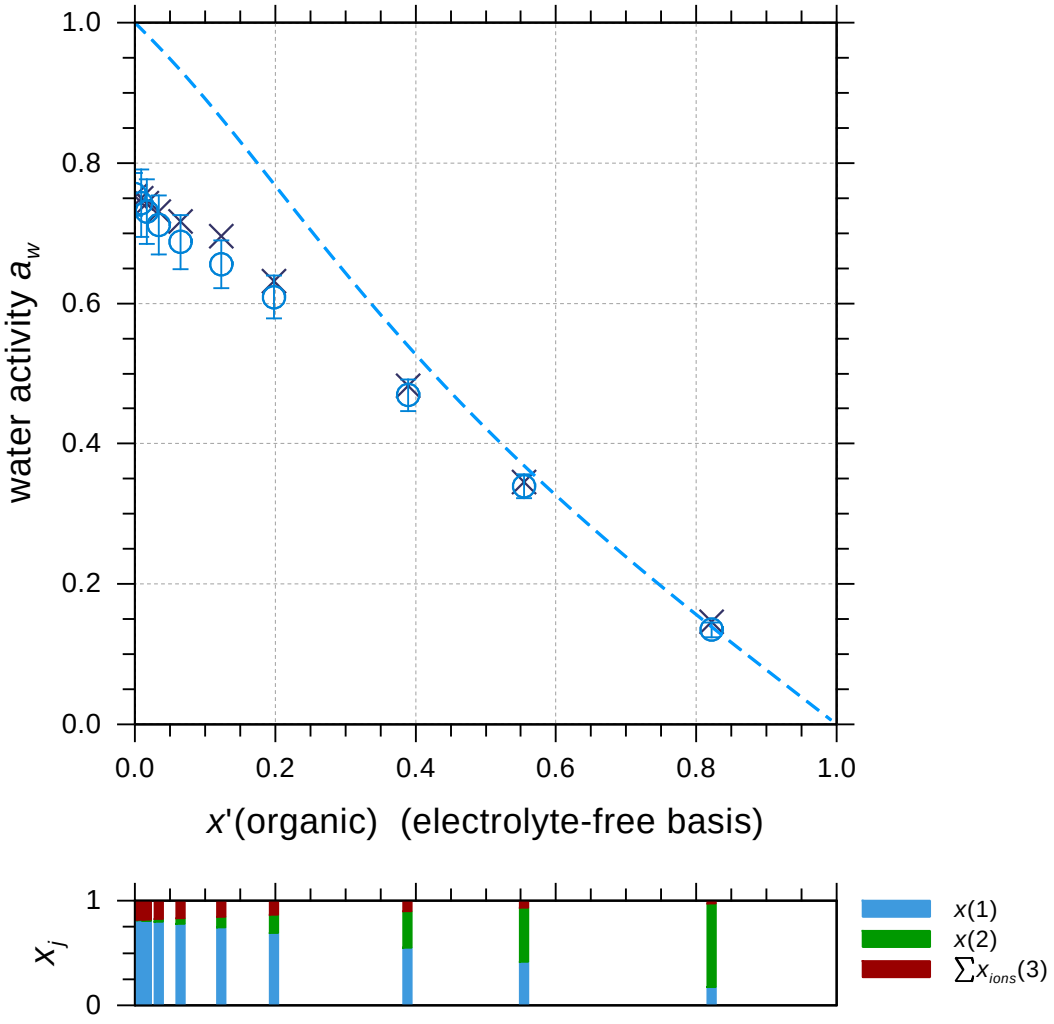


initial weighting of dataset:
$w^{init}(0023)$ = 0.000
dataset contribution to F_{obj}:
fval(0023) = 0.0000E+00
rel. contribution = 0.0000 %

Fig. S0139 (AIOMFAC_output_0024)

H_2O (1) + Glycerol (2) + NaCl (3)

Temperature: 298 K

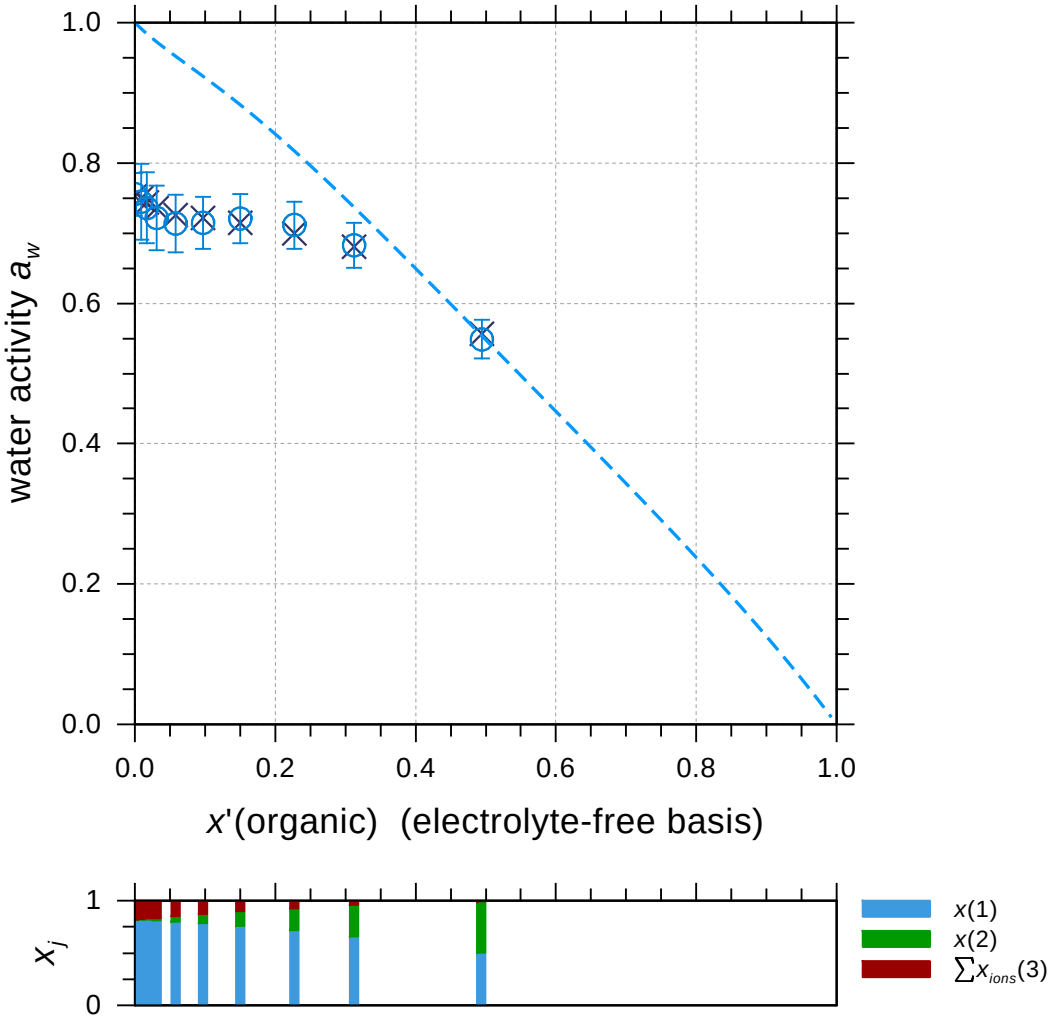


initial weighting of dataset:
$w^{init}(0024)$ = 2.000
dataset contribution to F_{obj}:
fval(0024) = 2.5327E-02
rel. contribution = 0.0120 %

Fig. S0140 (AIOMFAC_output_0025)

H_2O (1) + 1,4-Butanediol (2) + NaCl (3)

Temperature: 298 K

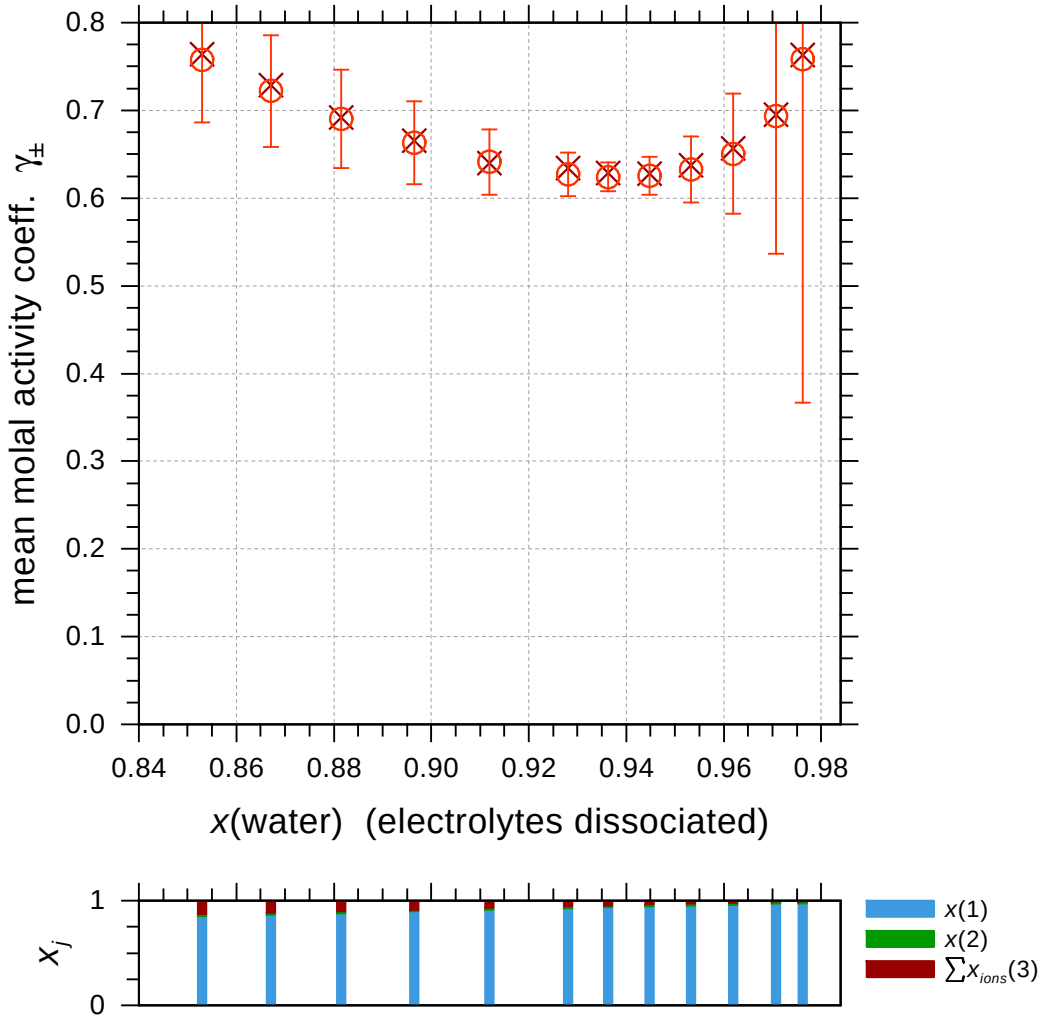


initial weighting of dataset:
$w^{init}(0025)$ = 2.000
dataset contribution to F_{obj}:
fval(0025) = 2.6950E-03
rel. contribution = 0.0013 %

Fig. S0141 (AIOMFAC_output_0034)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K

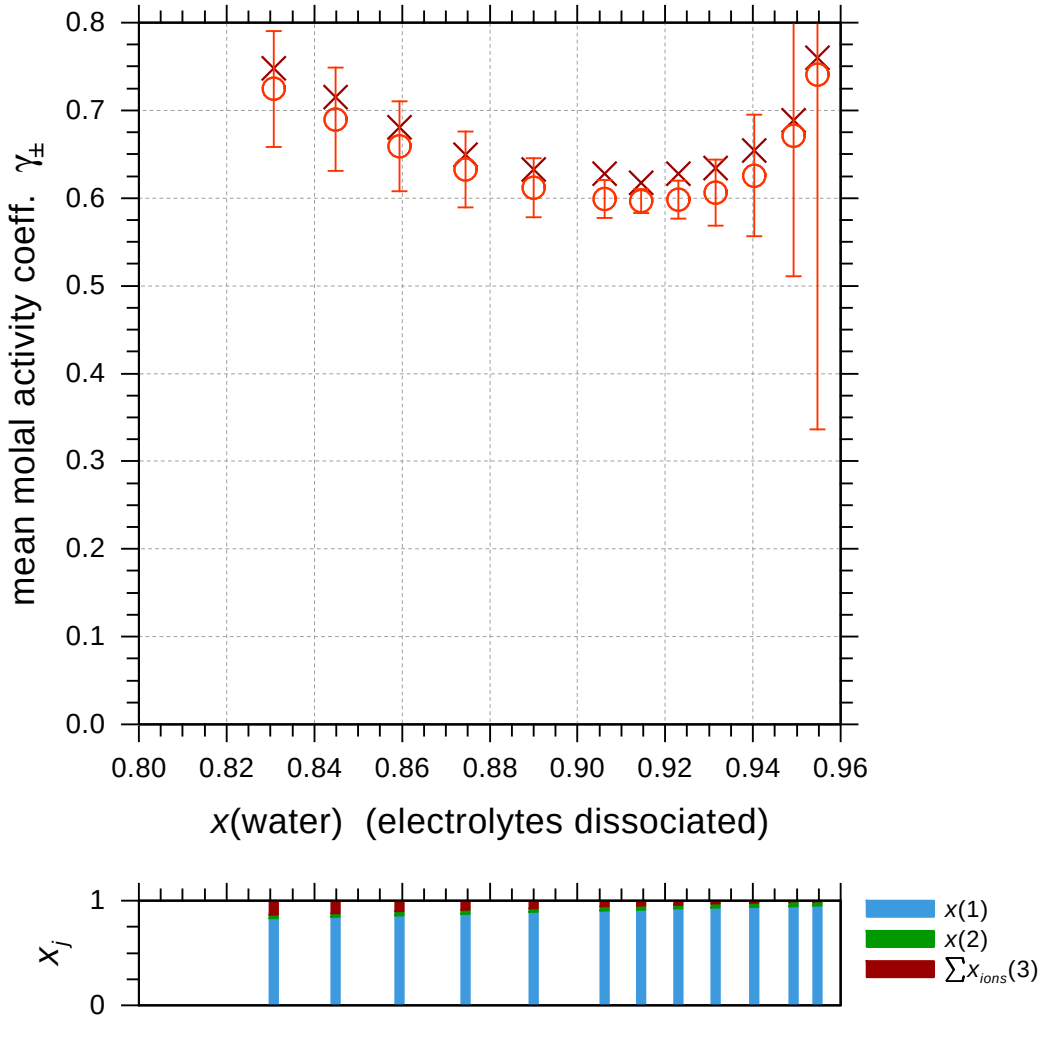


initial weighting of dataset:
$w^{init}(0034)$ = 2.000
dataset contribution to F_{obj}:
fval(0034) = 8.1937E-04
rel. contribution = 0.0004 %

Fig. S0142 (AIOMFAC_output_0035)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K

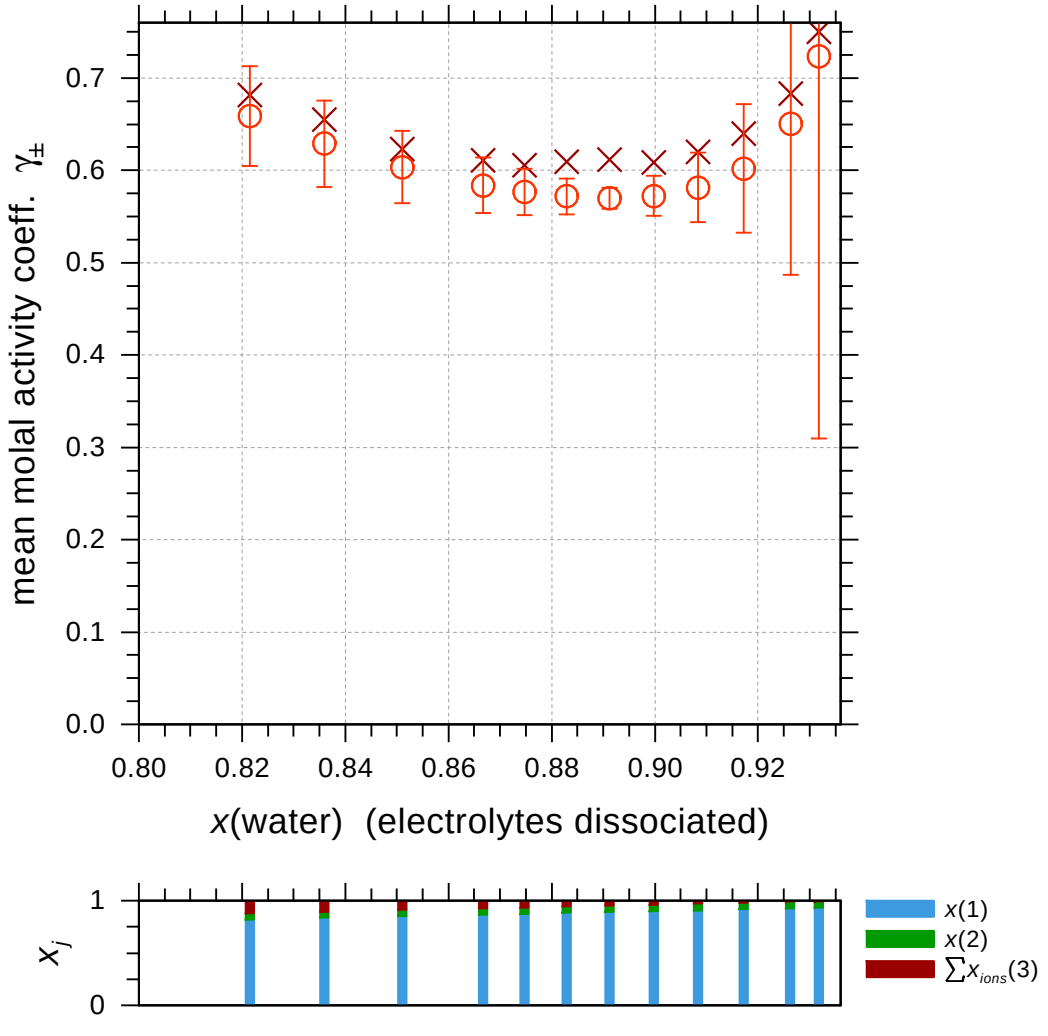


initial weighting of dataset:
$w^{init}(0035)$ = 2.000
dataset contribution to F_{obj}:
fval(0035) = 2.2290E-02
rel. contribution = 0.0106 %

Fig. S0143 (AIOMFAC_output_0036)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K

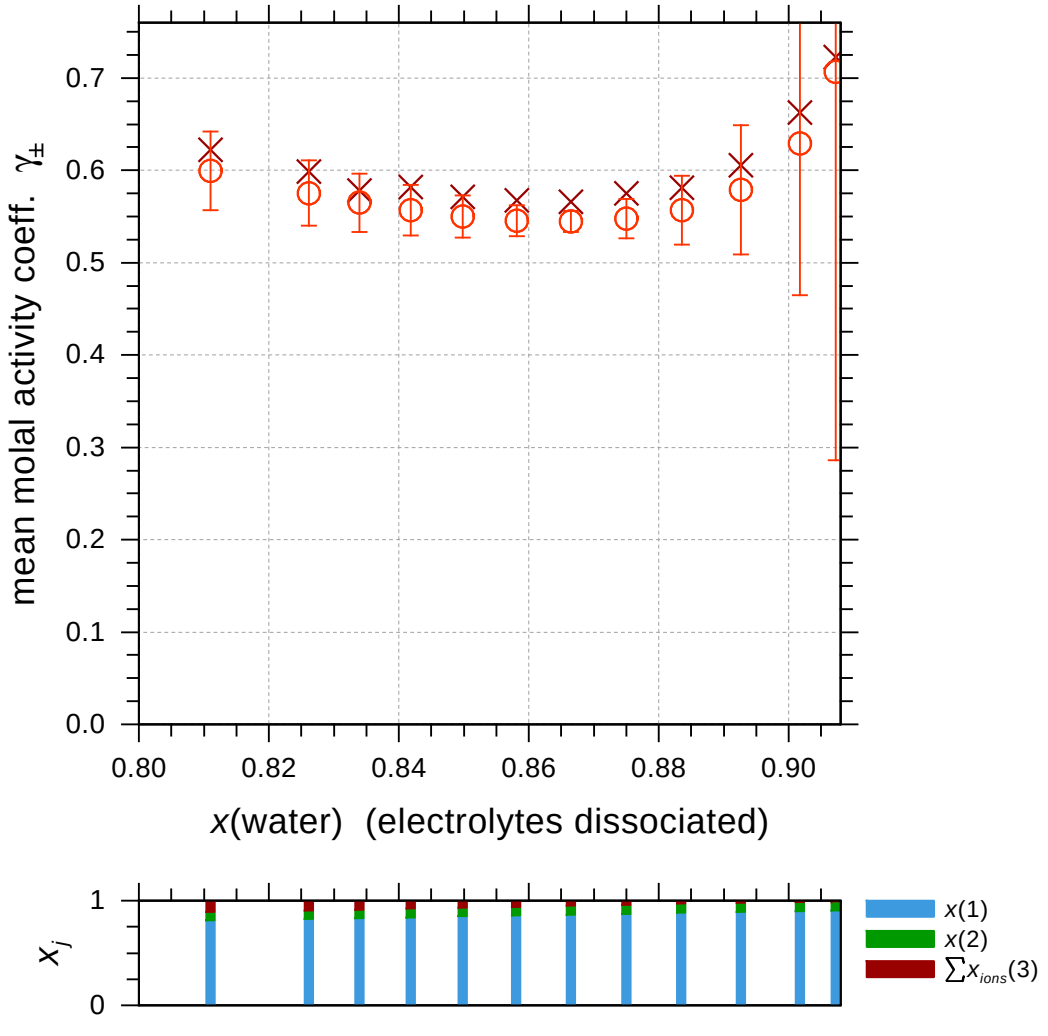


initial weighting of dataset:
$w^{init}(0036)$ = 2.000
dataset contribution to F_{obj}:
fval(0036) = 4.5065E-02
rel. contribution = 0.0214 %

Fig. S0144 (AIOMFAC_output_0037)

H_2O (1) + Ethanol (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:
w^{init}(0037) = 2.000
dataset contribution to F_{obj}:
fval(0037) = 2.6314E-02
rel. contribution = 0.0125 %

Fig. S0145 (AIOMFAC_output_0046)

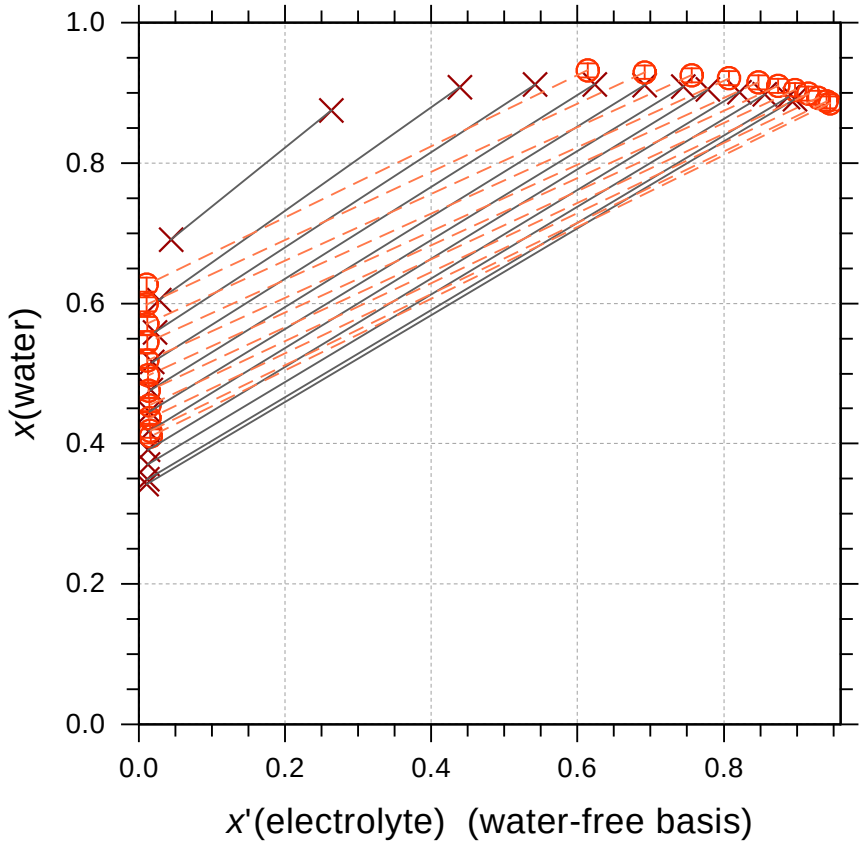
H_2O (1) + 1-Propanol (2) + NaCl (3)

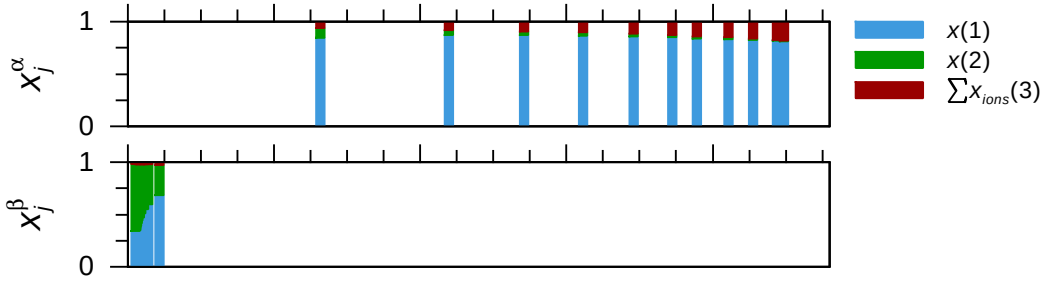
Temperature: 298 K

left y-axis:

× NaCl_1-PrOH_LLE_Santis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0046) = 1.000

dataset contribution to F_{obj}:

fval(0046) = 4.4931E-01

rel. contribution = 0.2137 %

Fig. S0145a (AIOMFAC_output_0046)

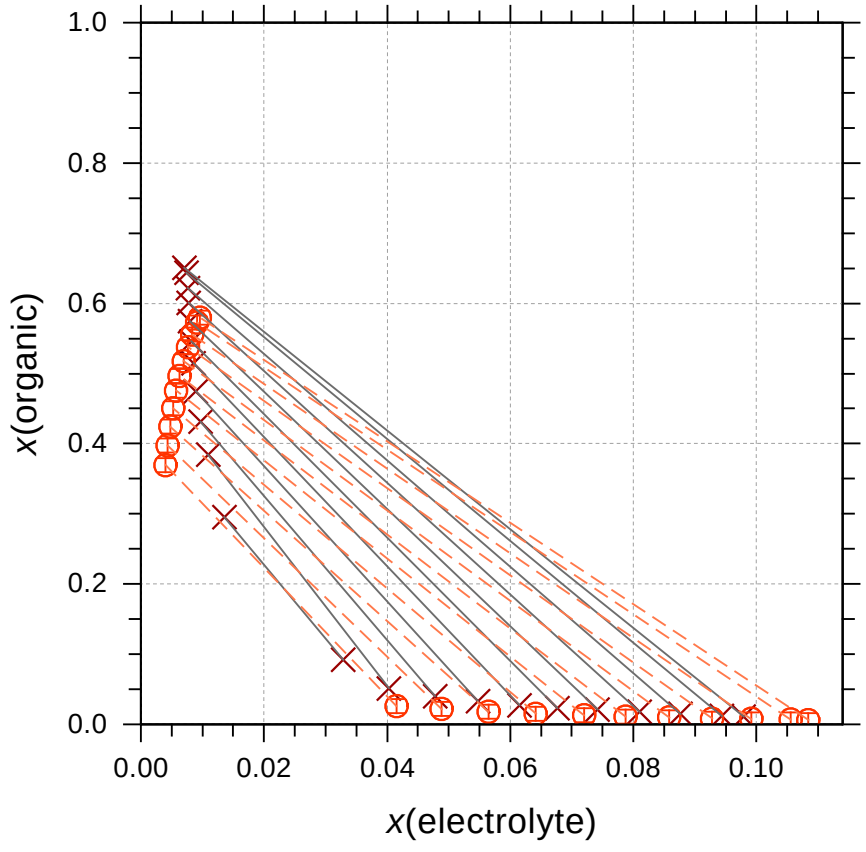
H_2O (1) + 1-Propanol (2) + NaCl (3)

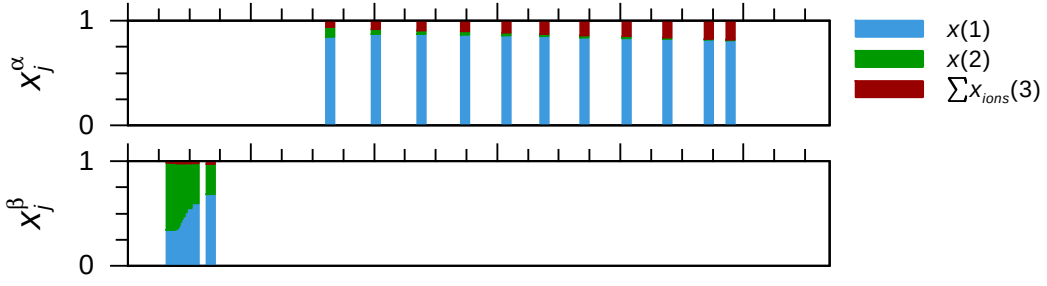
Temperature: 298 K

left y-axis:

× NaCl_1-PrOH_LLE_Santis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0046)$ = 1.000

dataset contribution to F_{obj}:

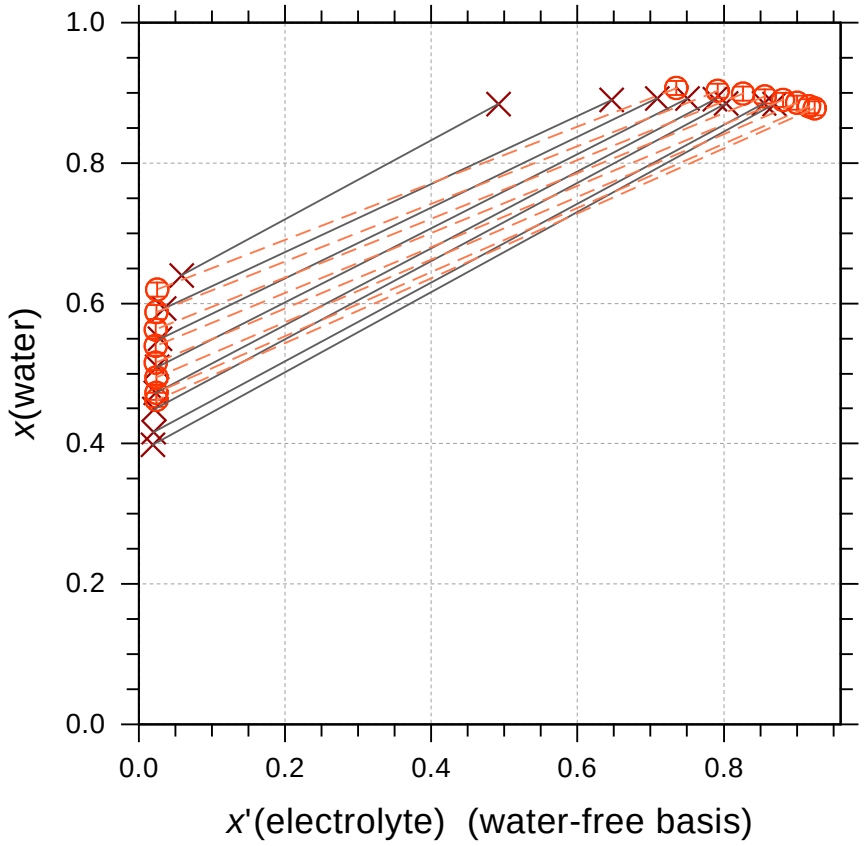
fval(0046) = 4.4931E-01

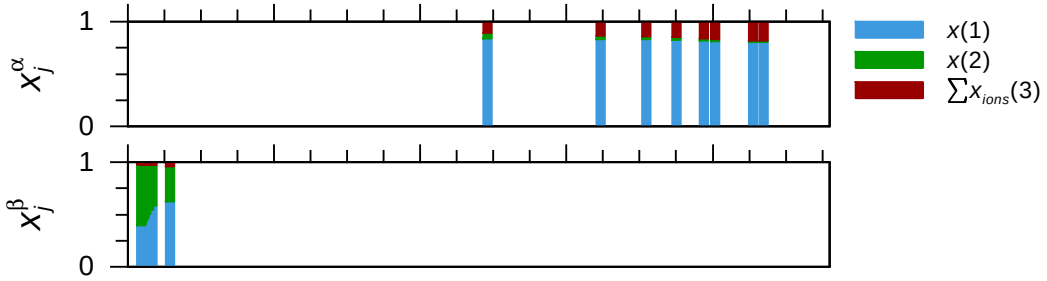
rel. contribution = 0.2137 %

Fig. S0146 (AIOMFAC_output_0047)

H_2O (1) + 2-Propanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_2-PrOH_LLE_Santis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0047)$ = 1.000

dataset contribution to F_{obj}:

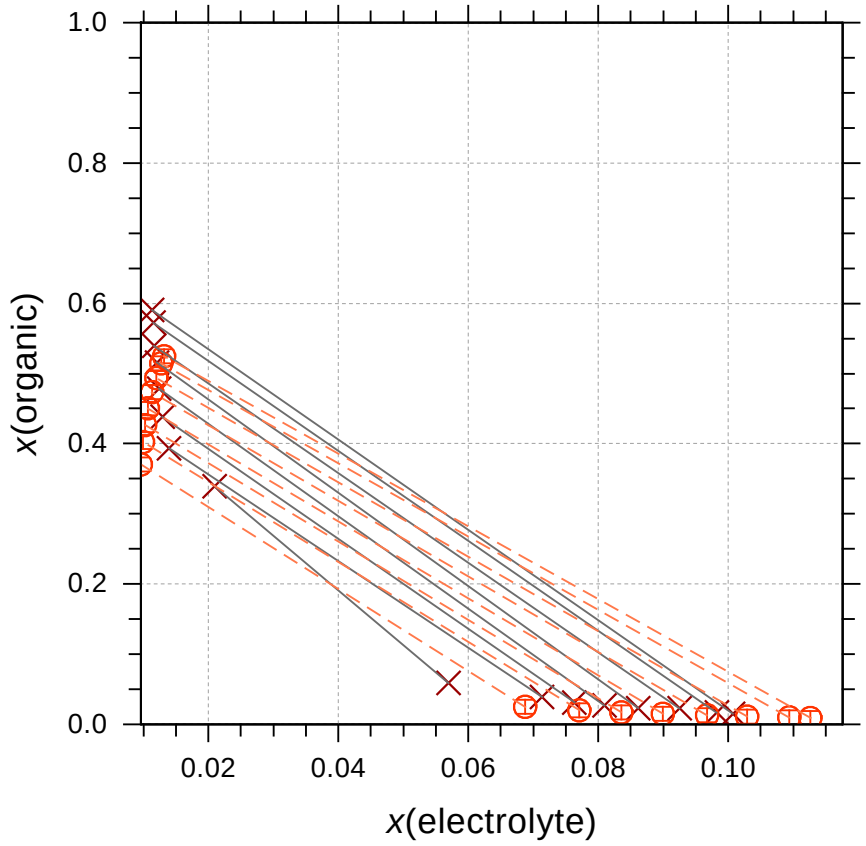
fval(0047) = 3.1567E-01

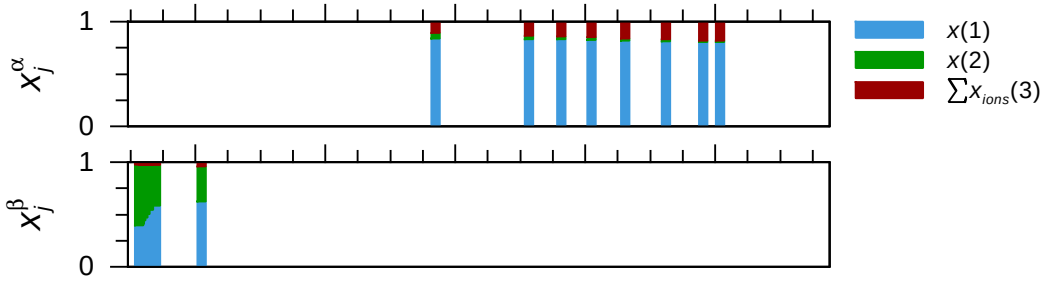
rel. contribution = 0.1501 %

Fig. S0146a (AIOMFAC_output_0047)

H_2O (1) + 2-Propanol (2) + NaCl (3)

Temperature: 298 K





initial weighting of dataset:
w^{init}(0047) = 1.000
dataset contribution to F_{obj}:
fval(0047) = 3.1567E-01
rel. contribution = 0.1501 %

Fig. S0147 (AIOMFAC_output_0048)

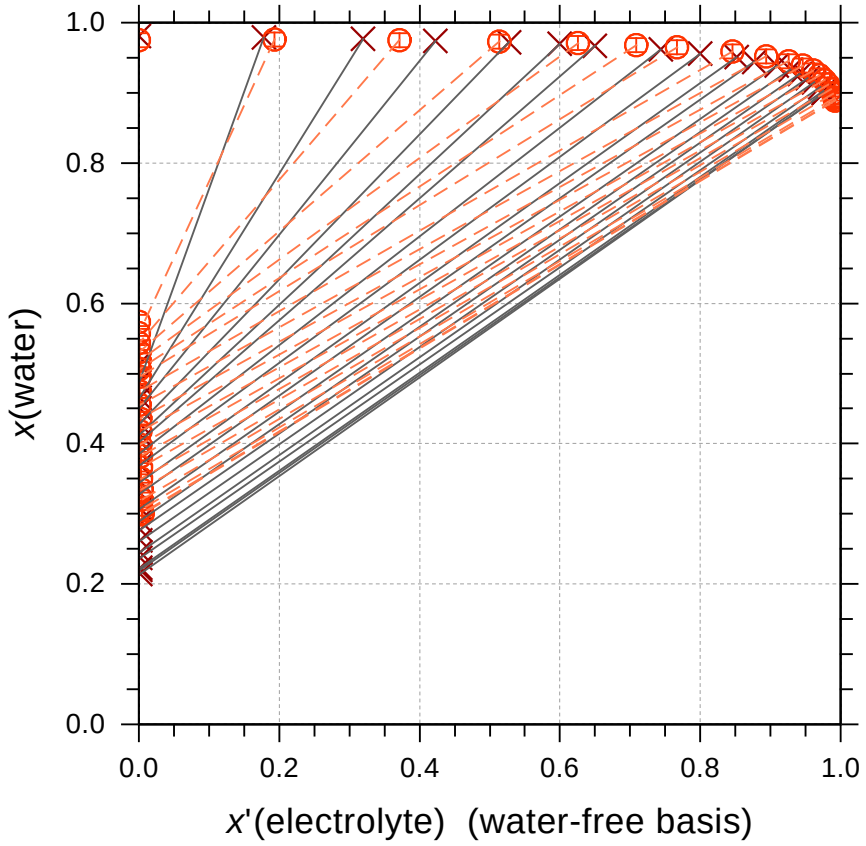
H_2O (1) + 1-Butanol (2) + NaCl (3)

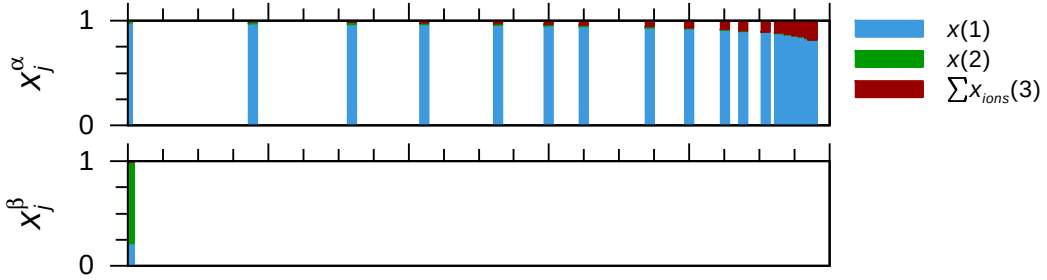
Temperature: 298 K

left y-axis:

× NaCl_1-BuOH_LLE_Santis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0048)$ = 1.000

dataset contribution to F_{obj}:

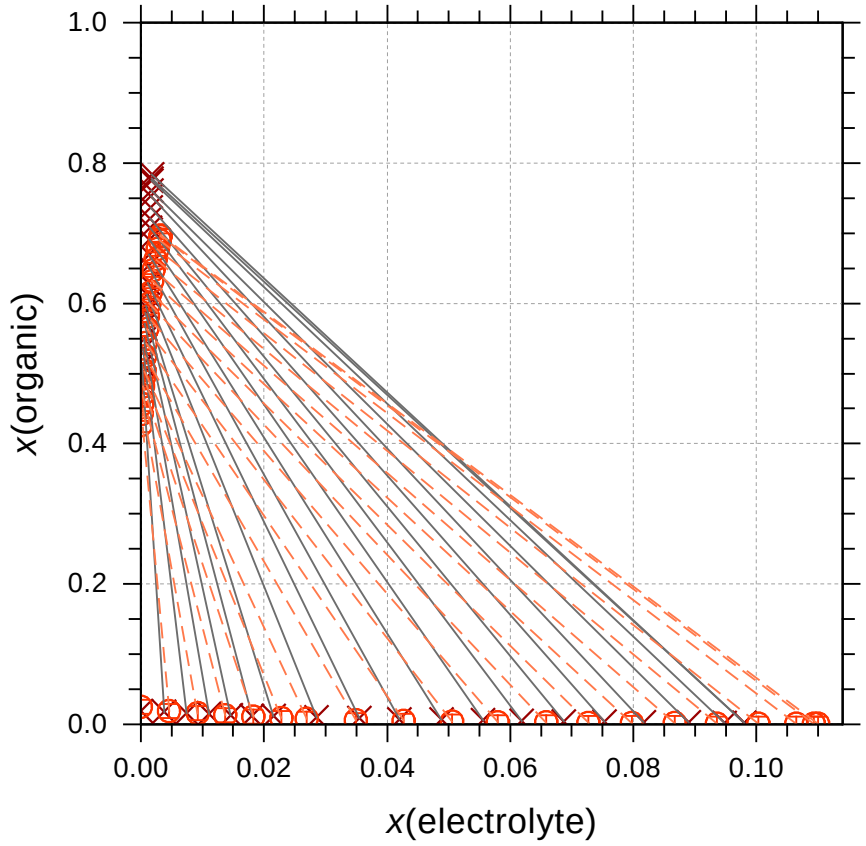
fval(0048) = 1.2396E-01

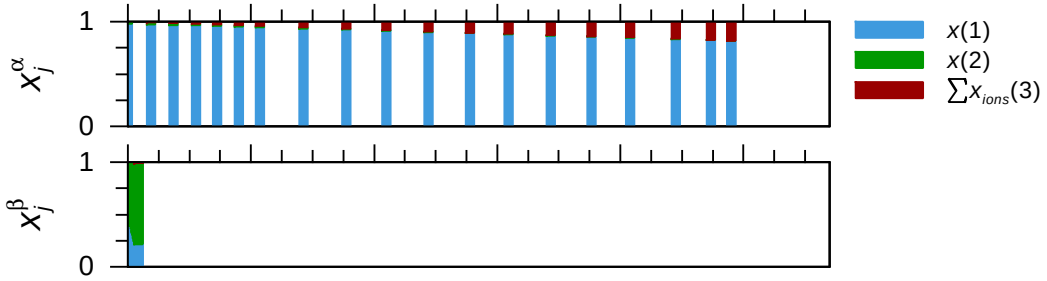
rel. contribution = 0.0589 %

Fig. S0147a (AIOMFAC_output_0048)

H_2O (1) + 1-Butanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_1-BuOH_LLE_Santis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0048) = 1.000

dataset contribution to F_{obj}:

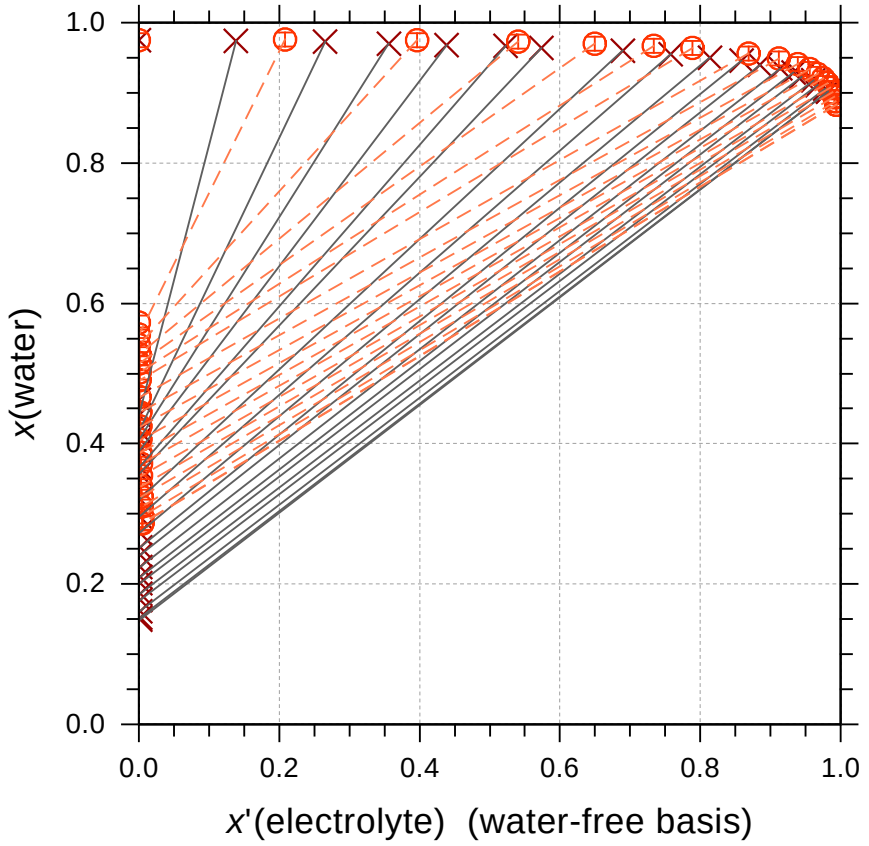
fval(0048) = 1.2396E-01

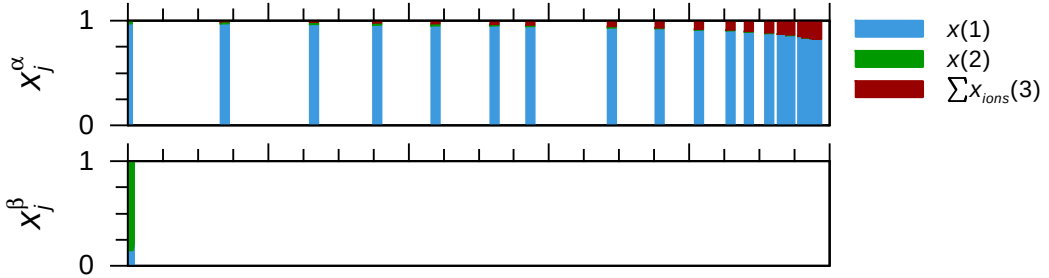
rel. contribution = 0.0589 %

Fig. S0148 (AIOMFAC_output_0049)

H_2O (1) + Isobutanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_iso-BuOH_LLE_Santis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0049) = 1.000

dataset contribution to F_{obj}:

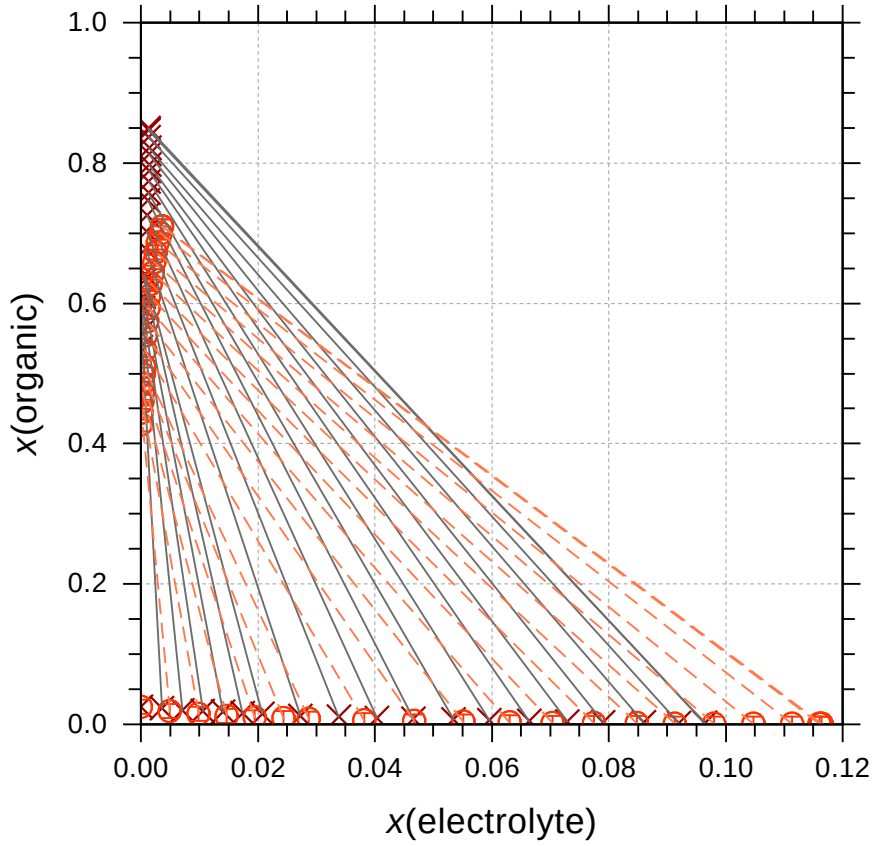
fval(0049) = 3.0845E-01

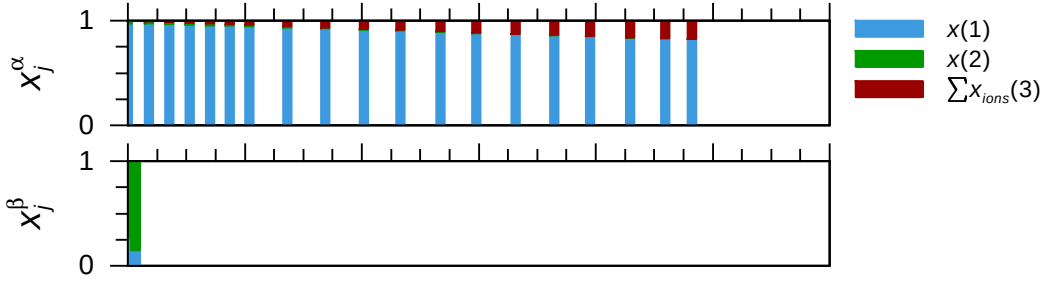
rel. contribution = 0.1467 %

Fig. S0148a (AIOMFAC_output_0049)

H_2O (1) + Isobutanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_iso-BuOH_LLE_Santis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0049)$ = 1.000

dataset contribution to F_{obj}:

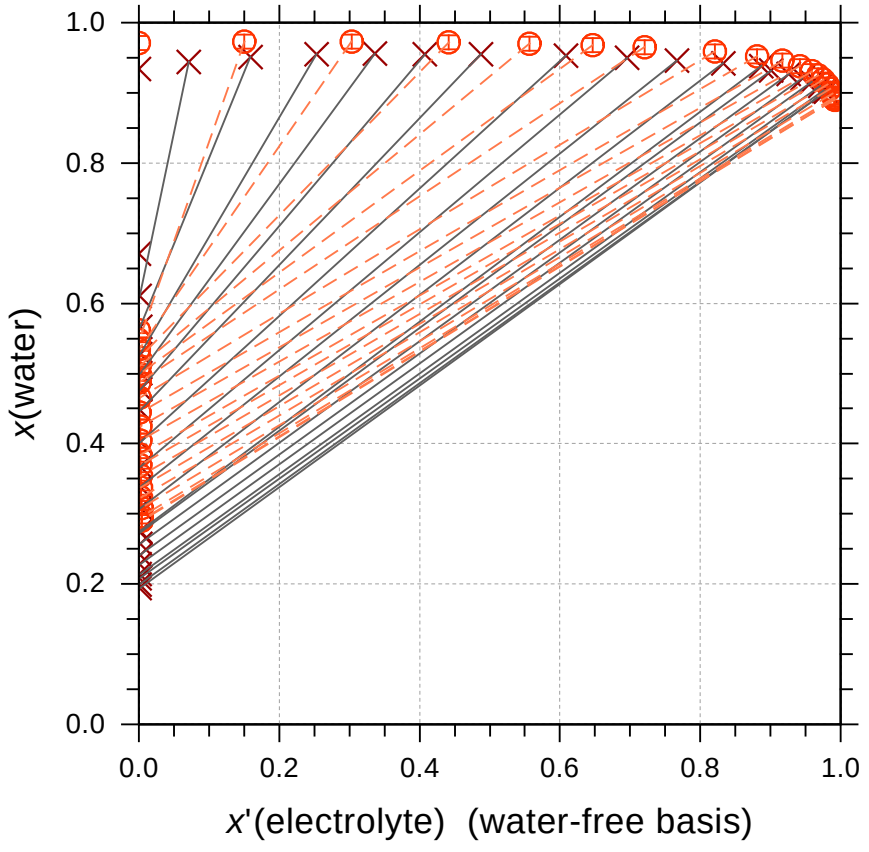
fval(0049) = 3.0845E-01

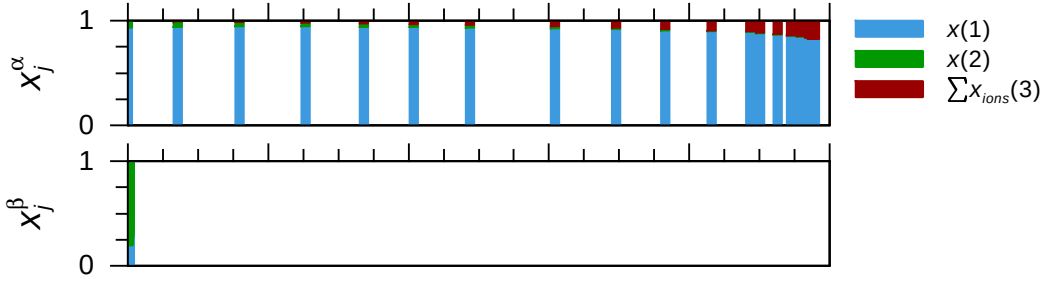
rel. contribution = 0.1467 %

Fig. S0149 (AIOMFAC_output_0050)

H_2O (1) + 2-Butanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_2-BuOH_LLE_Santis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0050)$ = 1.000

dataset contribution to F_{obj}:

fval(0050) = 3.2729E-01

rel. contribution = 0.1556 %

Fig. S0149a (AIOMFAC_output_0050)

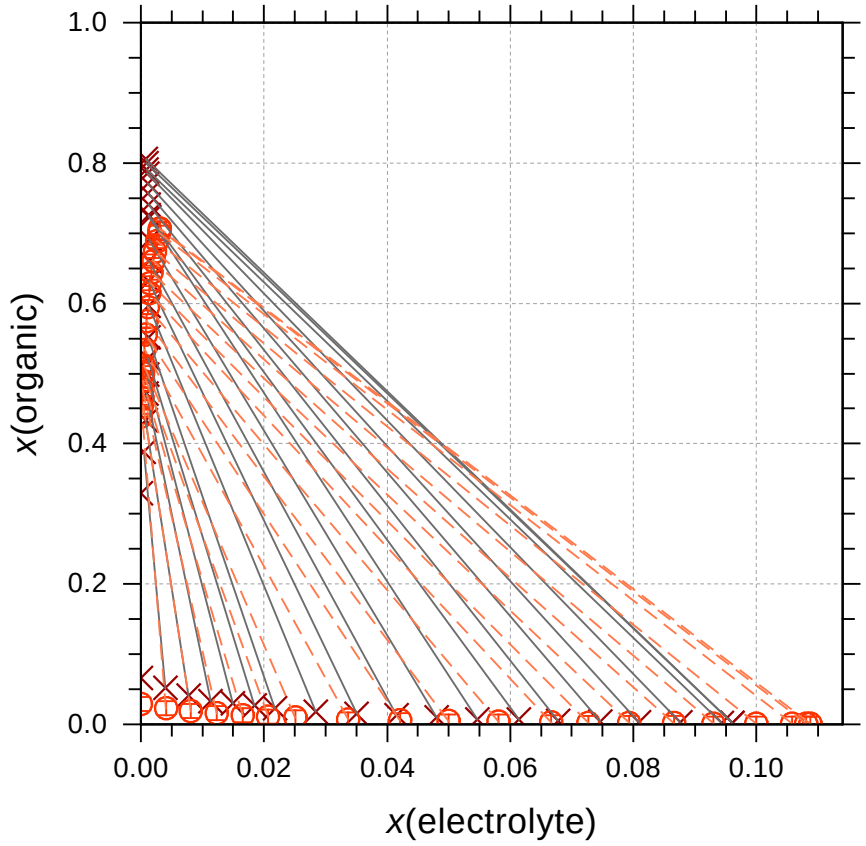
H_2O (1) + 2-Butanol (2) + NaCl (3)

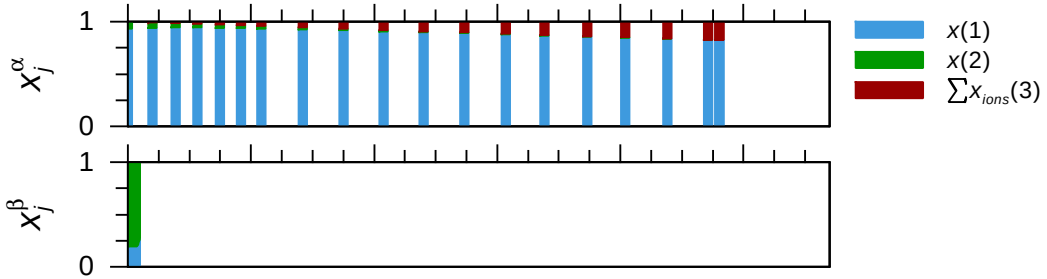
Temperature: 298 K

left y-axis:

× NaCl_2-BuOH_LLE_Santis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0050)$ = 1.000

dataset contribution to F_{obj}:

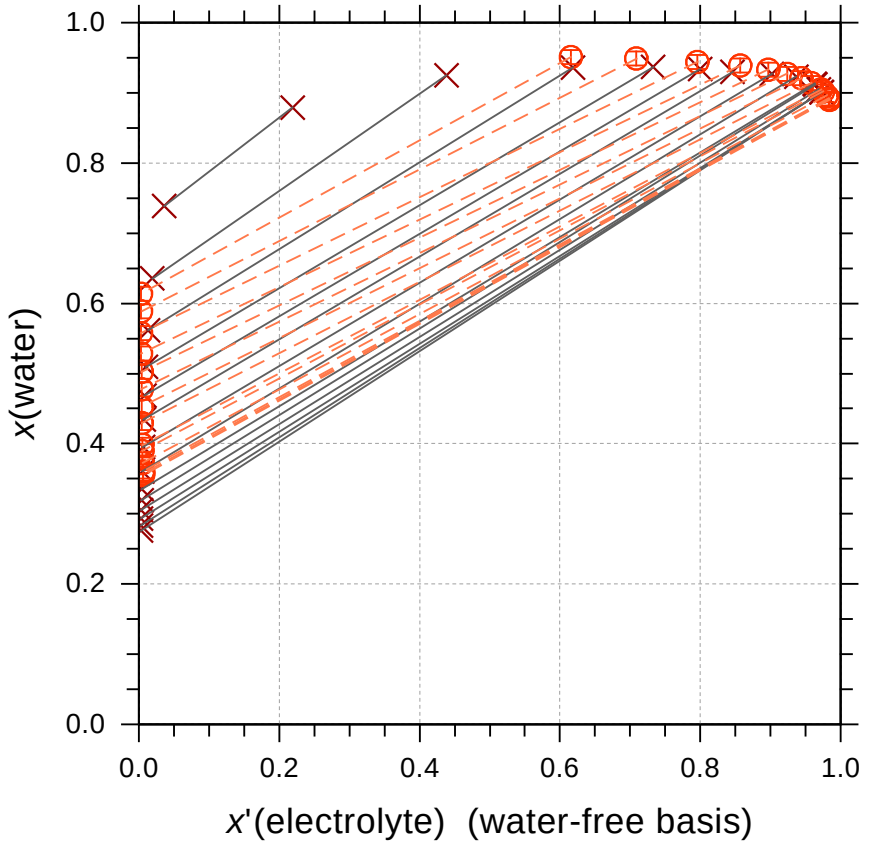
fval(0050) = 3.2729E-01

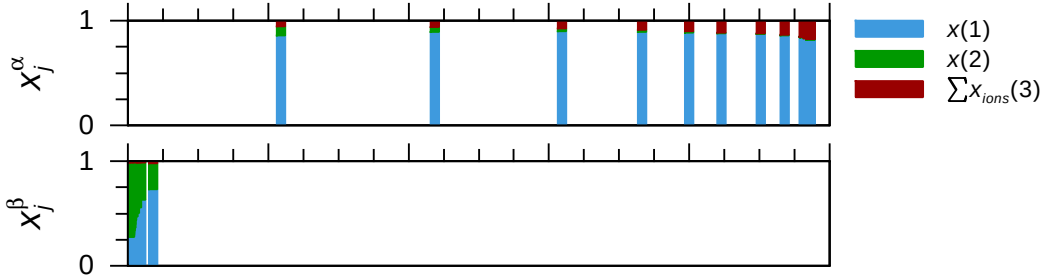
rel. contribution = 0.1556 %

Fig. S0150 (AIOMFAC_output_0051)

H_2O (1) + *tert*-Butanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_tert-BuOH_LLE_Santis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0051)$ = 1.000

dataset contribution to F_{obj}:

fval(0051) = 3.2279E-01

rel. contribution = 0.1535 %

Fig. S0150a (AIOMFAC_output_0051)

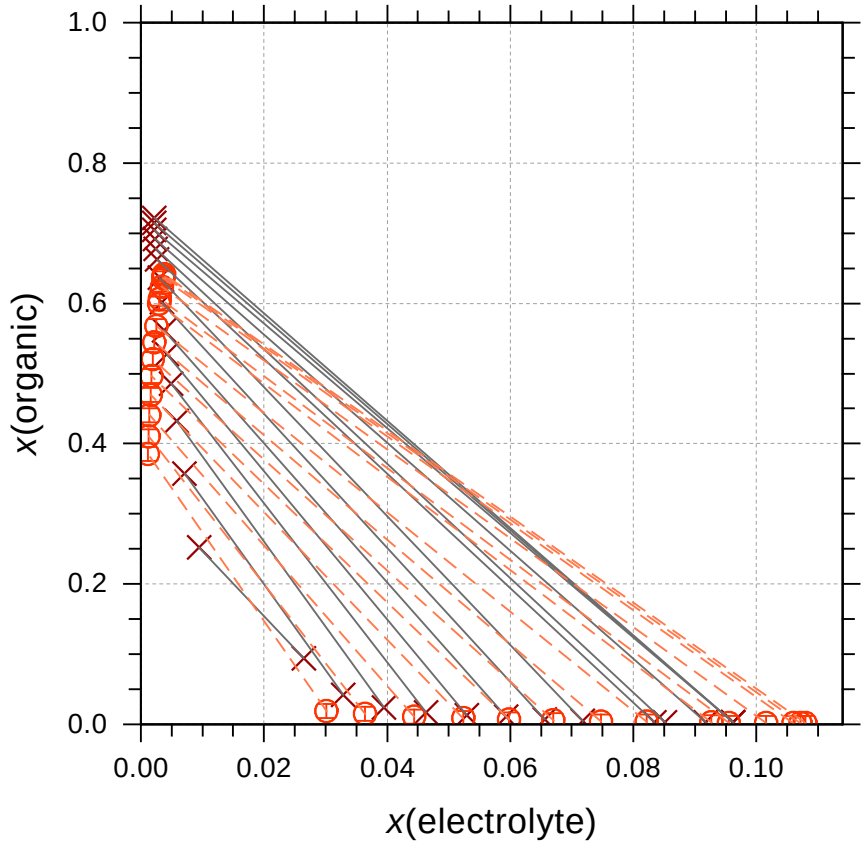
H_2O (1) + *tert*-Butanol (2) + NaCl (3)

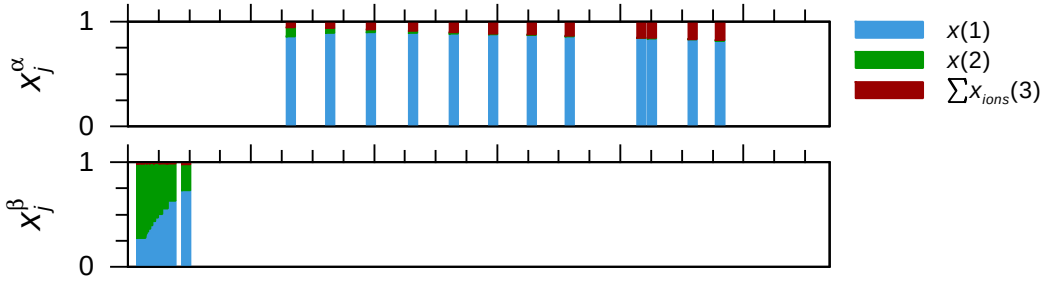
Temperature: 298 K

left y-axis:

× NaCl_tert-BuOH_LLE_Santis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0051) = 1.000

dataset contribution to F_{obj}:

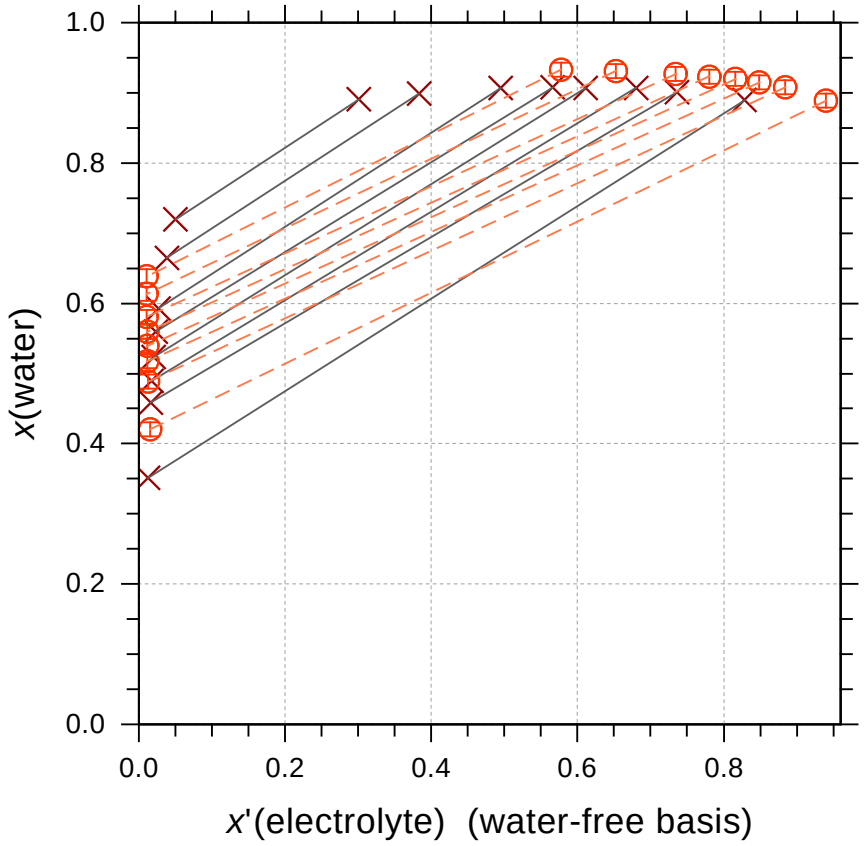
fval(0051) = 3.2279E-01

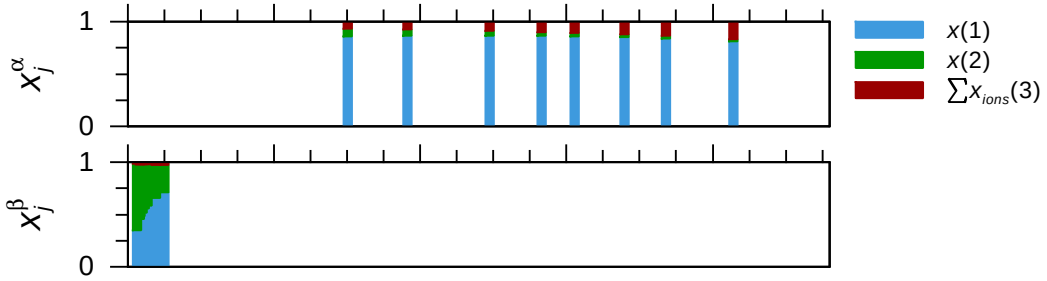
rel. contribution = 0.1535 %

Fig. S0151 (AIOMFAC_output_0052)

H_2O (1) + 1-Propanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_1-PrOH_LLE_Chou

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0052) = 1.000

dataset contribution to F_{obj}:

fval(0052) = 6.5865E-01

rel. contribution = 0.3132 %

Fig. S0151a (AIOMFAC_output_0052)

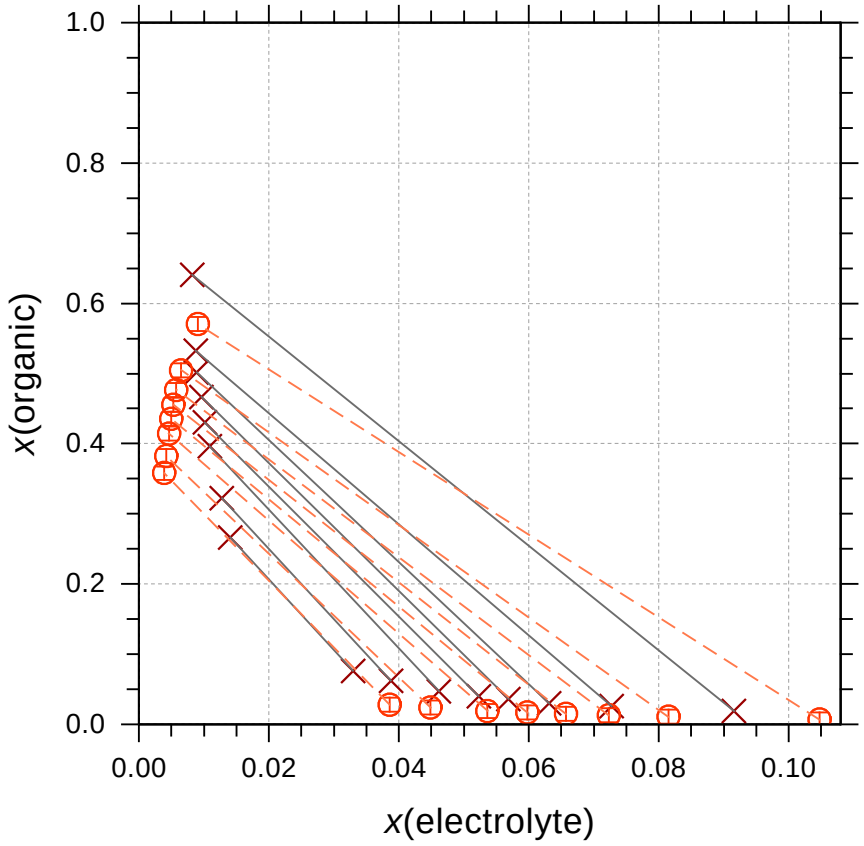
H_2O (1) + 1-Propanol (2) + NaCl (3)

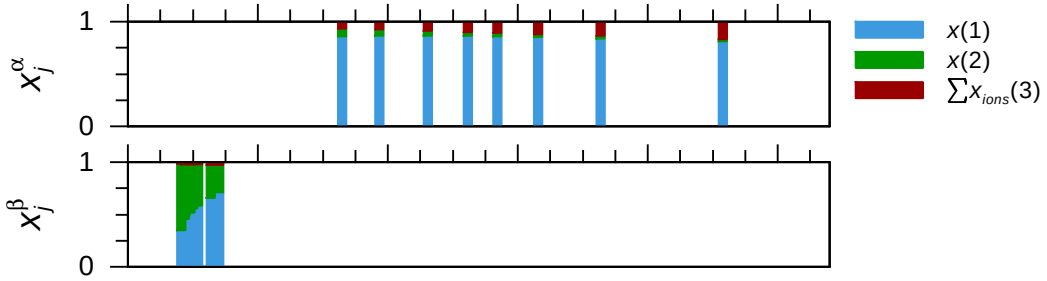
Temperature: 298 K

left y-axis:

× NaCl_1-PrOH_LLE_Chou

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0052)$ = 1.000

dataset contribution to F_{obj}:

fval(0052) = 6.5865E-01

rel. contribution = 0.3132 %

Fig. S0152 (AIOMFAC_output_0053)

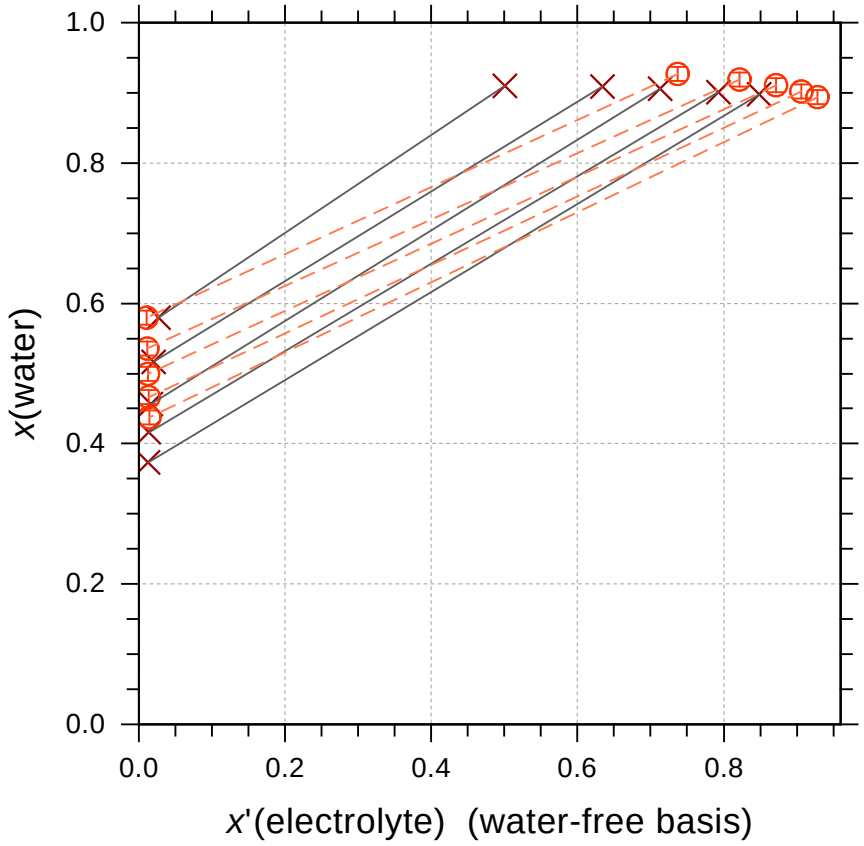
H_2O (1) + 1-Propanol (2) + NaCl (3)

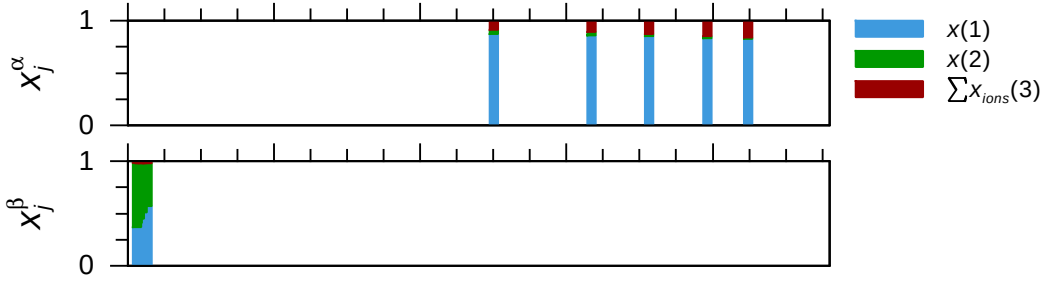
Temperature: 298 K

left y-axis:

× NaCl_1-PrOH_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0053)$ = 1.000

dataset contribution to F_{obj}:

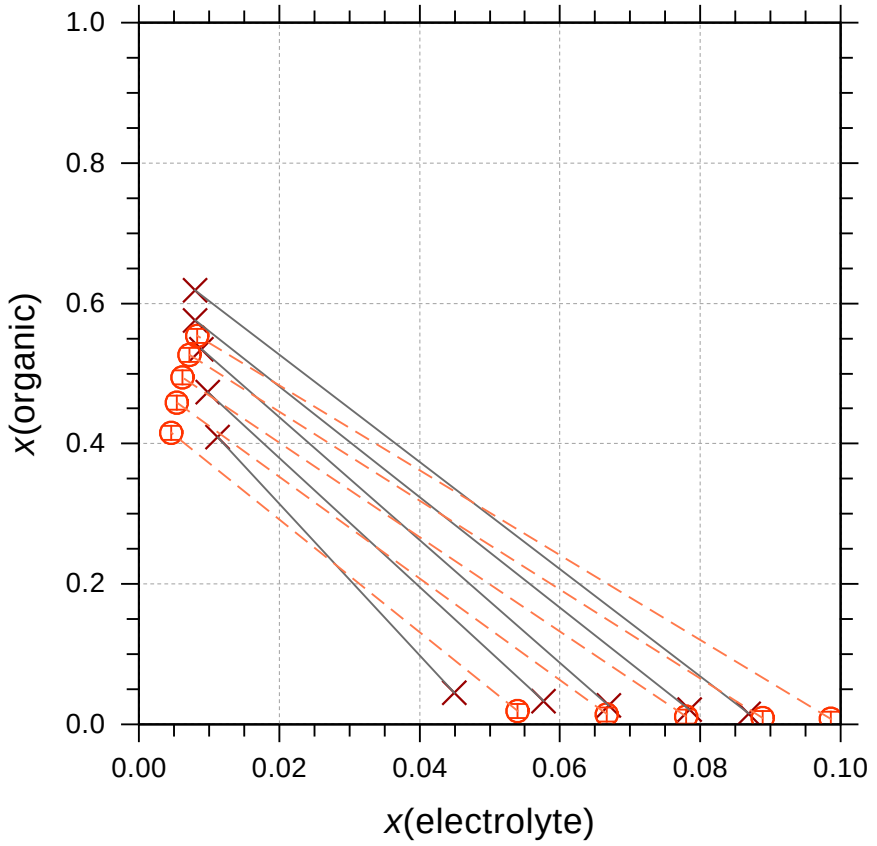
fval(0053) = 6.1731E-01

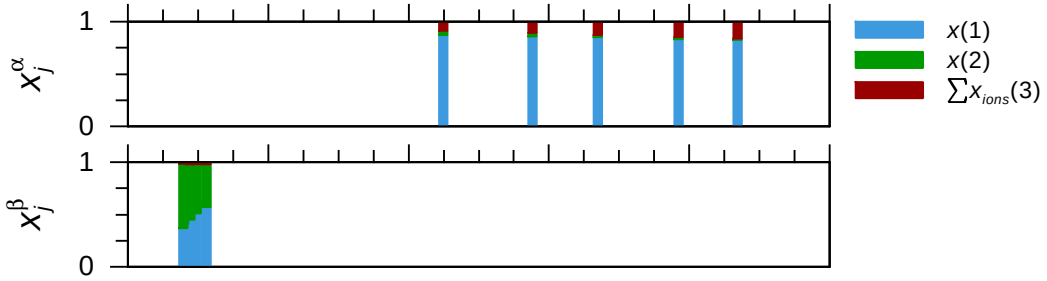
rel. contribution = 0.2936 %

Fig. S0152a (AIOMFAC_output_0053)

H_2O (1) + 1-Propanol (2) + NaCl (3)

Temperature: 298 K



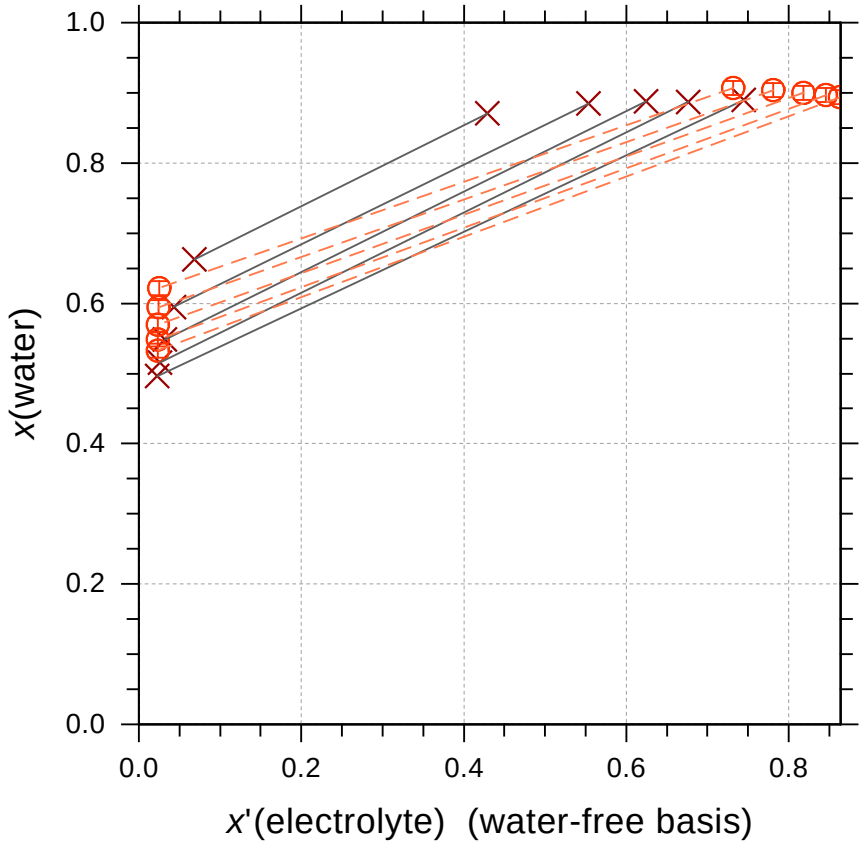


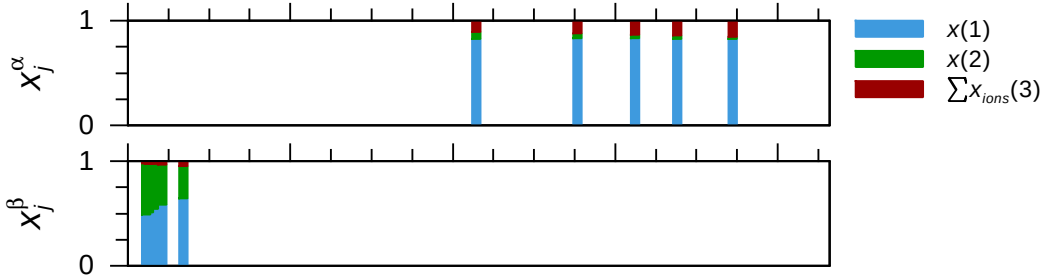
initial weighting of dataset:
$w^{init}(0053)$ = 1.000
dataset contribution to F_{obj}:
fval(0053) = 6.1731E-01
rel. contribution = 0.2936 %

Fig. S0153 (AIOMFAC_output_0054)

H_2O (1) + 2-Propanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_2-PrOH_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0054) = 1.000

dataset contribution to F_{obj}:

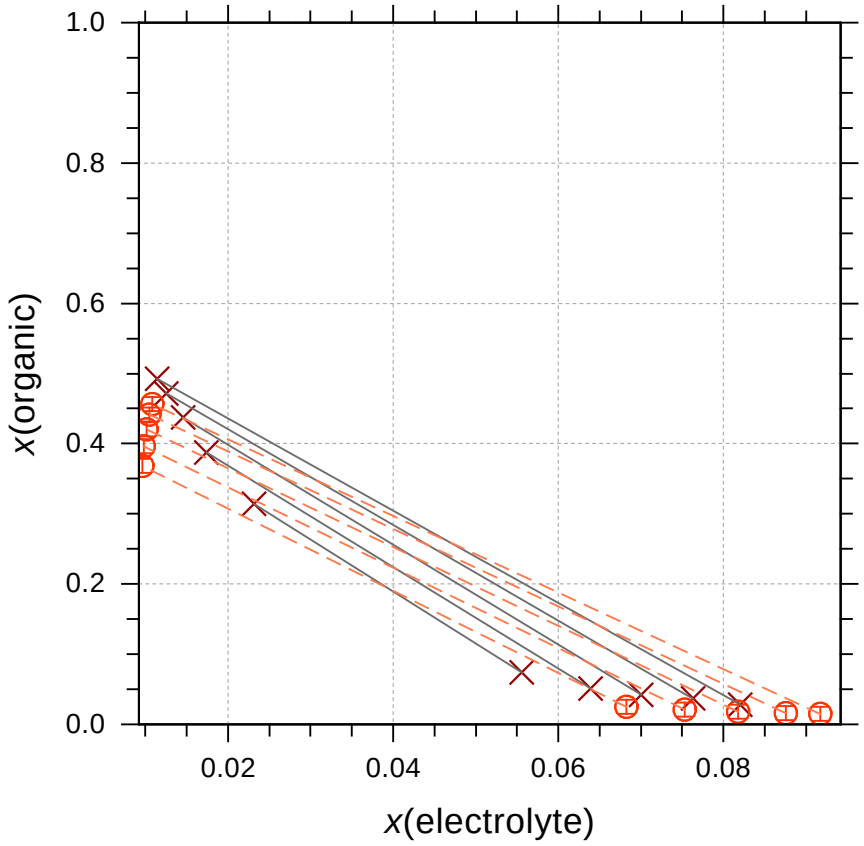
fval(0054) = 4.8392E-01

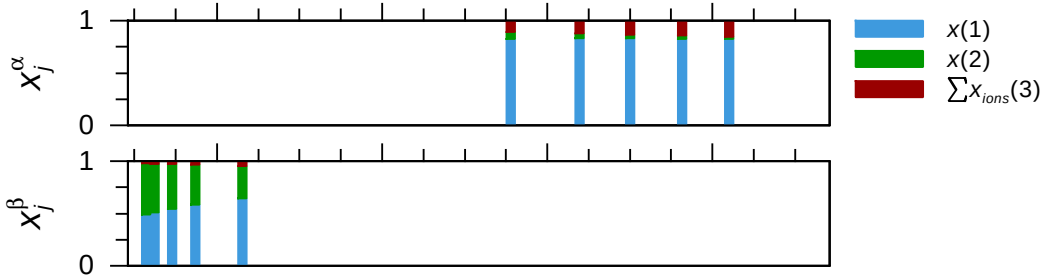
rel. contribution = 0.2301 %

Fig. S0153a (AIOMFAC_output_0054)

H_2O (1) + 2-Propanol (2) + NaCl (3)

Temperature: 298 K



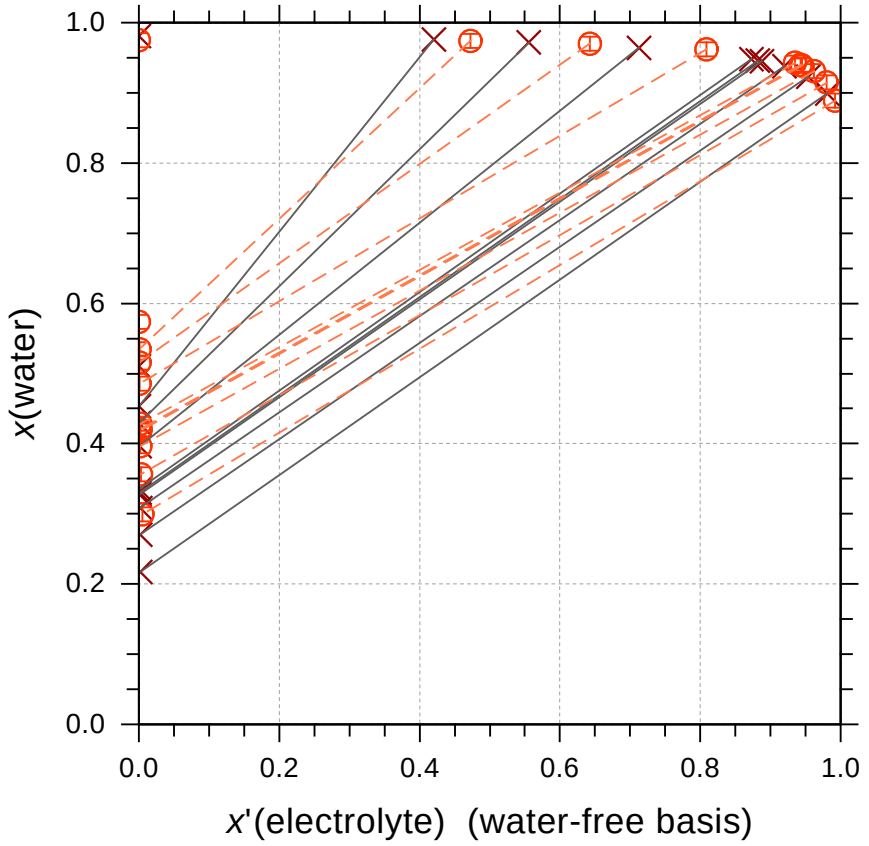


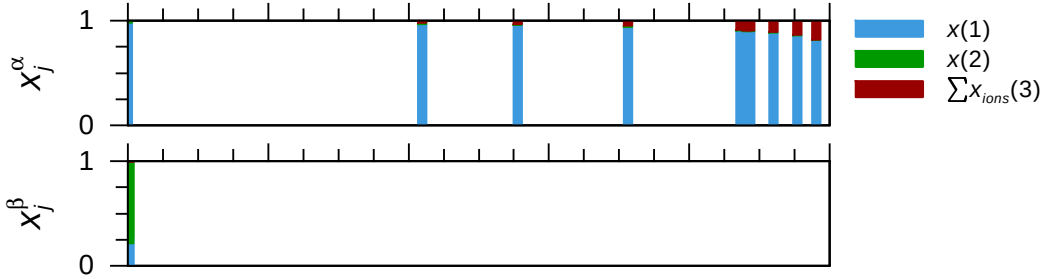
initial weighting of dataset:
w^{init}(0054) = 1.000
dataset contribution to F_{obj}:
fval(0054) = 4.8392E-01
rel. contribution = 0.2301 %

Fig. S0154 (AIOMFAC_output_0055)

H_2O (1) + 1-Butanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_1-BuOH_LLE_Li

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0055)$ = 1.000

dataset contribution to F_{obj}:

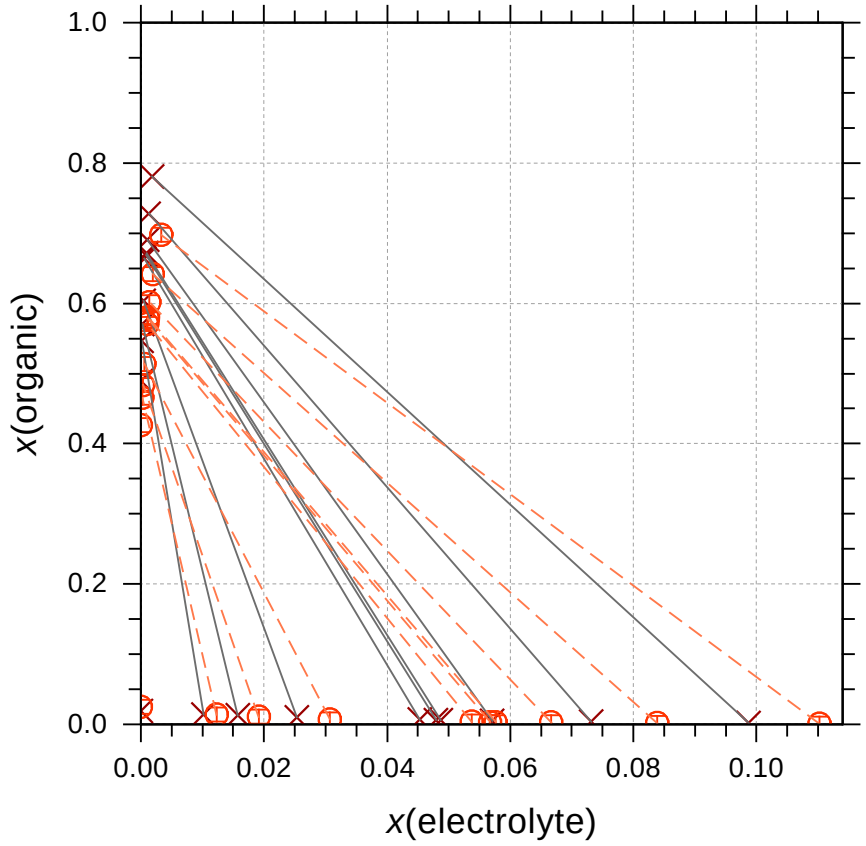
fval(0055) = 9.7787E-02

rel. contribution = 0.0465 %

Fig. S0154a (AIOMFAC_output_0055)

H_2O (1) + 1-Butanol (2) + NaCl (3)

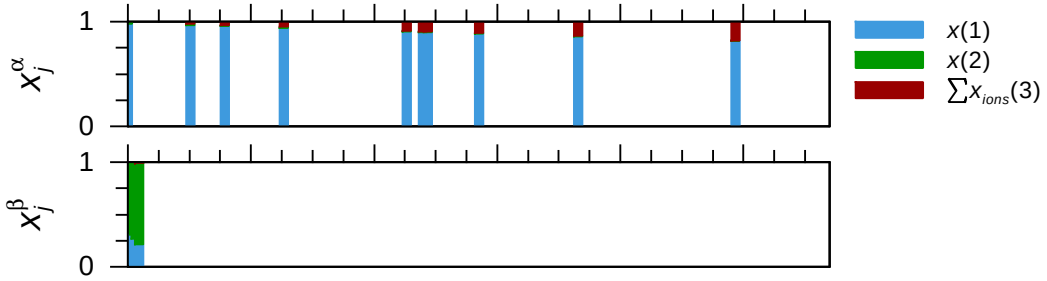
Temperature: 298 K



left y-axis:

× NaCl_1-BuOH_LLE_Li

○ AIOMFAC calc. LLE composition



initial weighting of dataset:

w^{init}(0055) = 1.000

dataset contribution to F_{obj}:

fval(0055) = 9.7787E-02

rel. contribution = 0.0465 %

Fig. S0155 (AIOMFAC_output_0056)

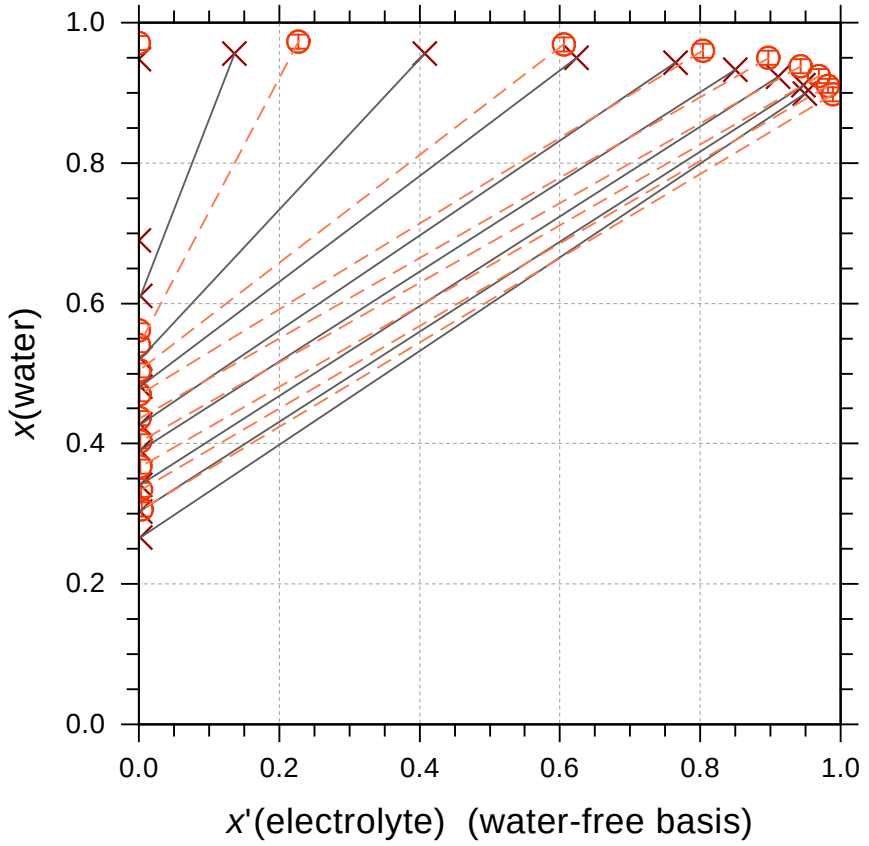
H_2O (1) + 2-Butanol (2) + NaCl (3)

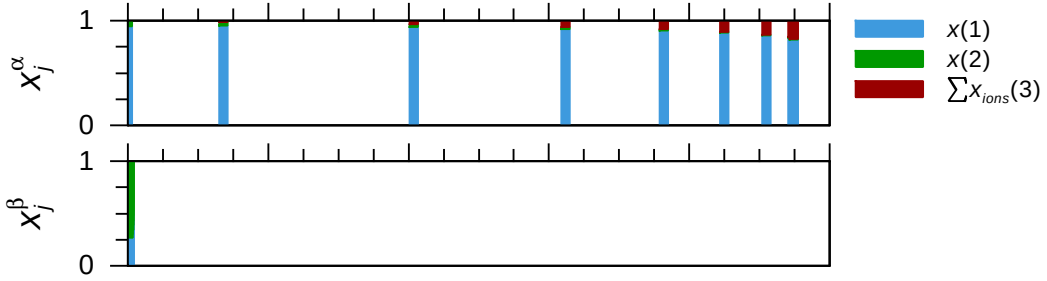
Temperature: 298 K

left y-axis:

× NaCl_2-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:
w^{init}(0056) = 1.000
dataset contribution to F_{obj}:
fval(0056) = 5.2718E-01
rel. contribution = 0.2507 %

Fig. S0155a (AIOMFAC_output_0056)

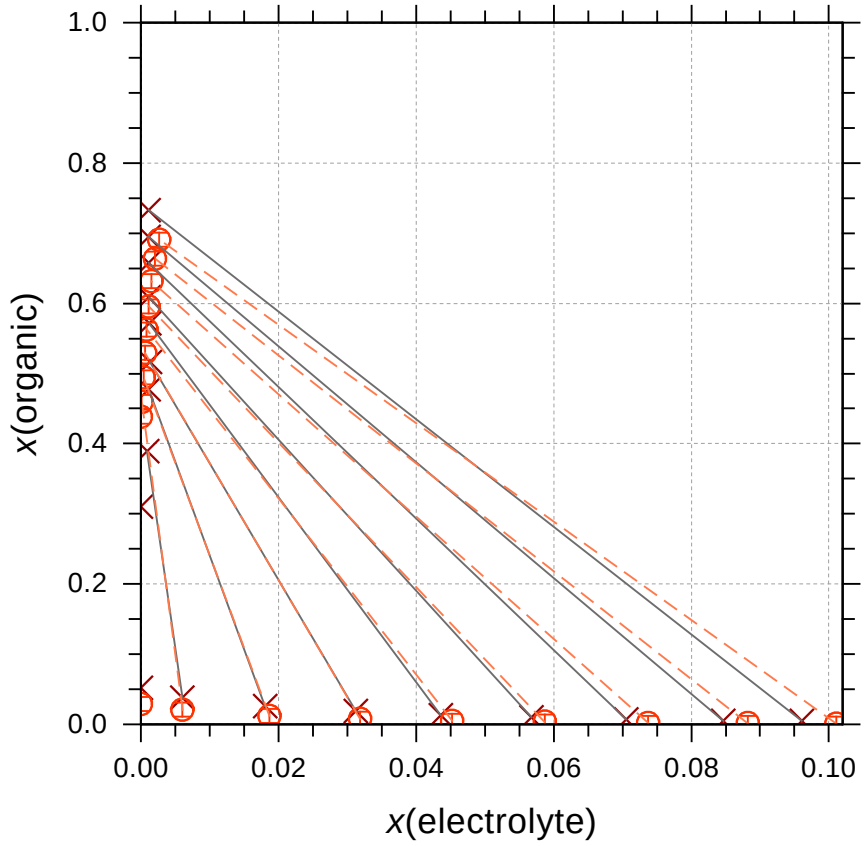
H_2O (1) + 2-Butanol (2) + NaCl (3)

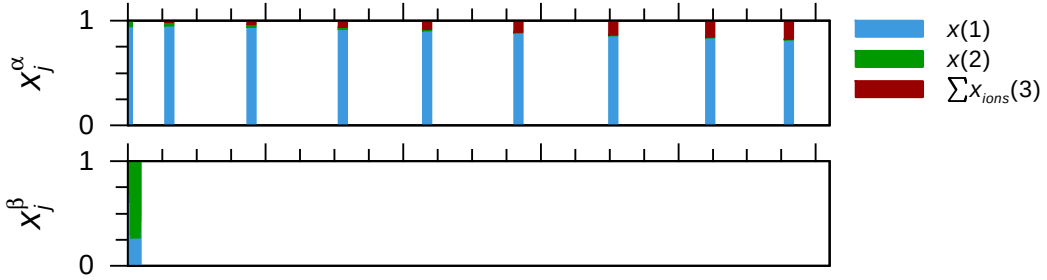
Temperature: 298 K

left y-axis:

× NaCl_2-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0056)$ = 1.000

dataset contribution to F_{obj}:

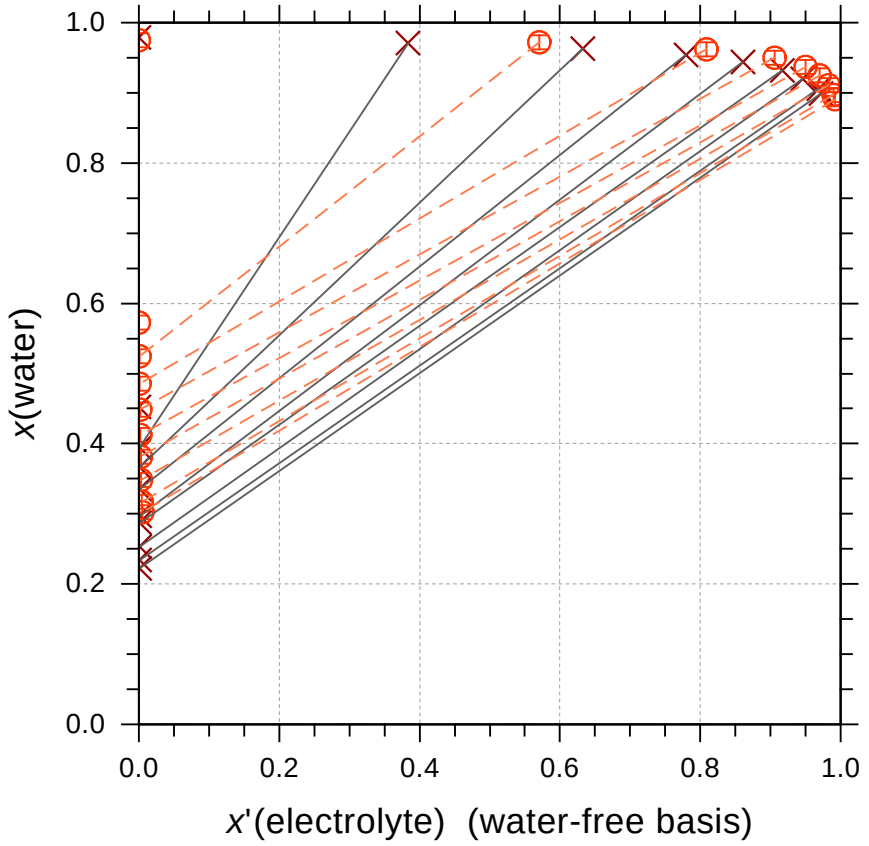
fval(0056) = 5.2718E-01

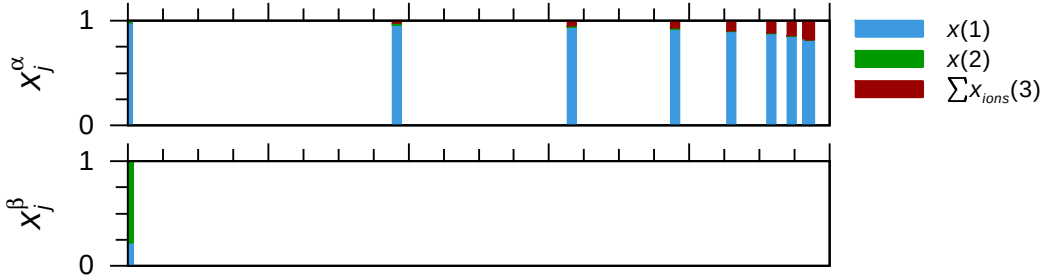
rel. contribution = 0.2507 %

Fig. S0156 (AIOMFAC_output_0057)

H_2O (1) + Isobutanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_iso-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0057) = 1.000

dataset contribution to F_{obj}:

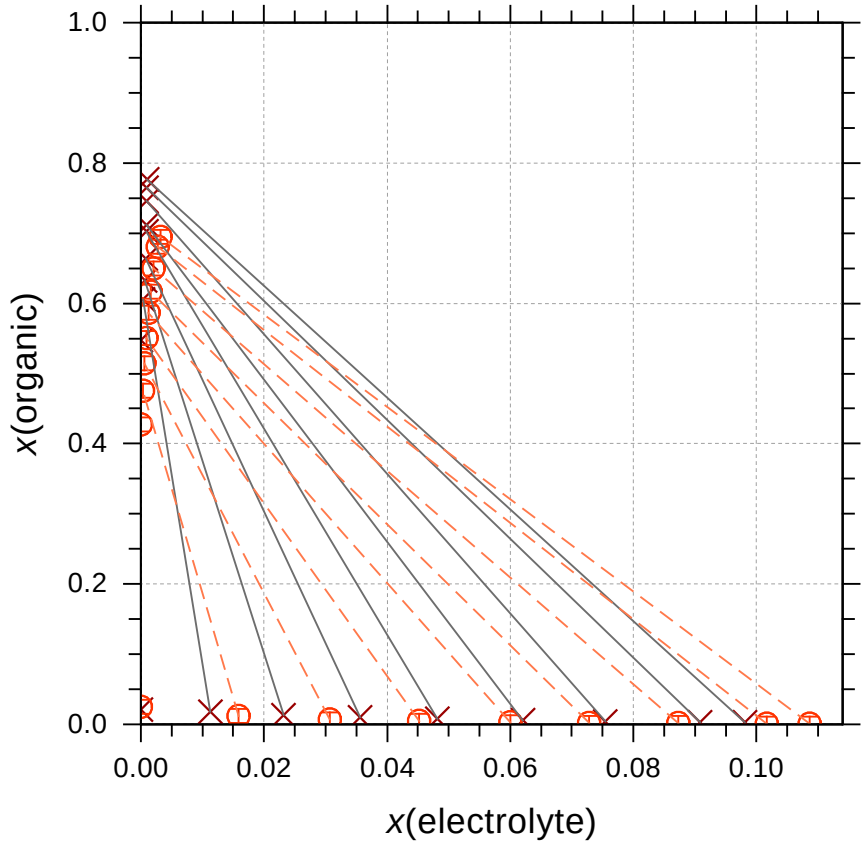
fval(0057) = 1.9471E-01

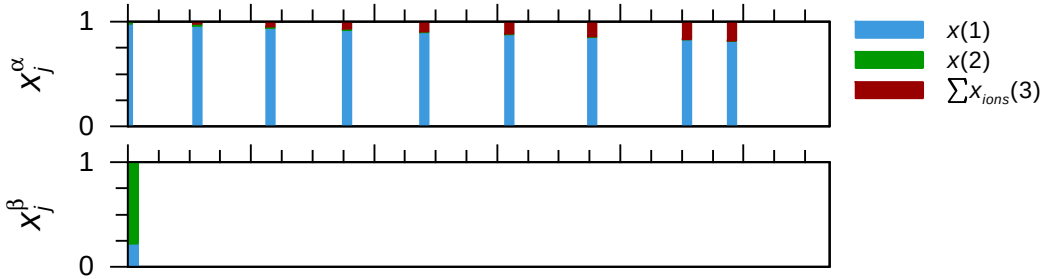
rel. contribution = 0.0926 %

Fig. S0156a (AIOMFAC_output_0057)

H_2O (1) + Isobutanol (2) + NaCl (3)

Temperature: 298 K



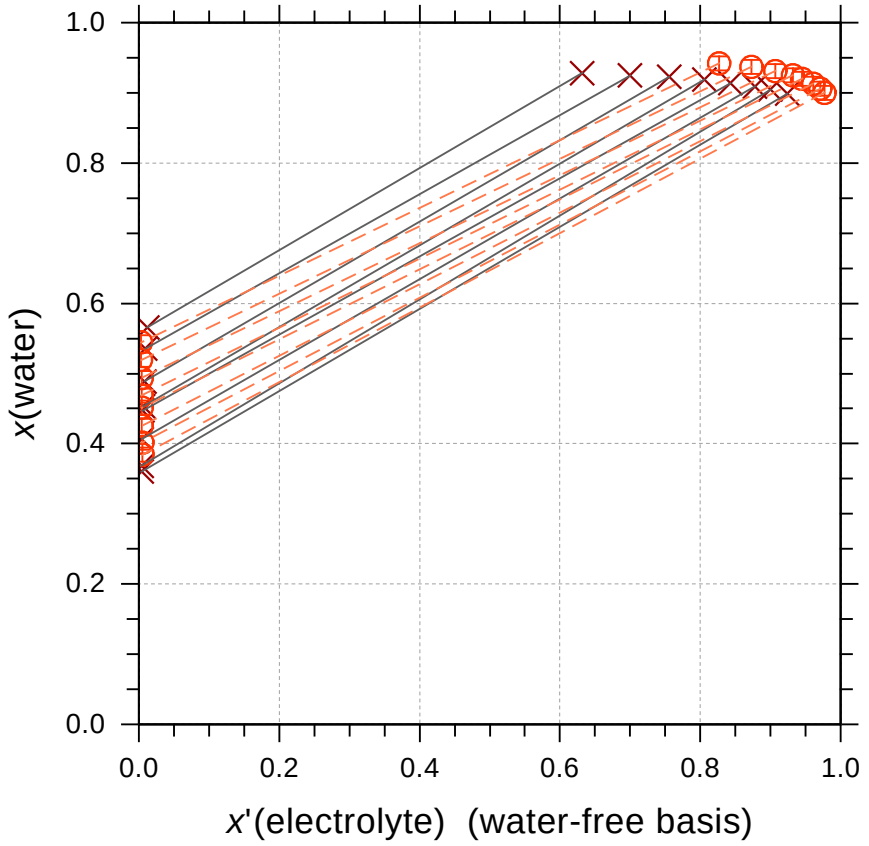


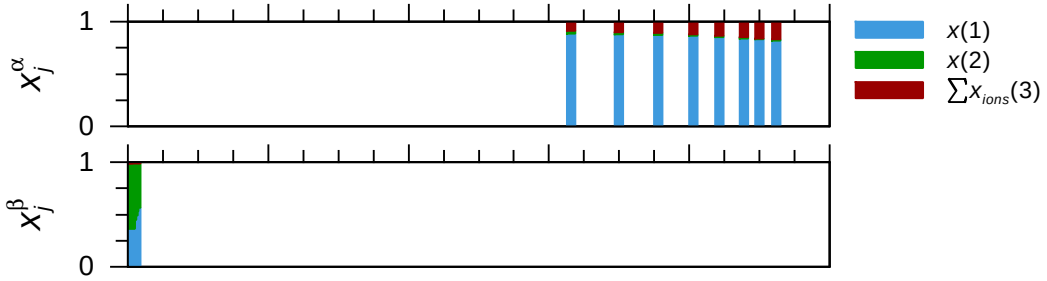
initial weighting of dataset:
w^{init}(0057) = 1.000
dataset contribution to F_{obj}:
fval(0057) = 1.9471E-01
rel. contribution = 0.0926 %

Fig. S0157 (AIOMFAC_output_0058)

H_2O (1) + *tert*-Butanol (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl_tert-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0058)$ = 1.000

dataset contribution to F_{obj}:

fval(0058) = 9.8986E-01

rel. contribution = 0.4707 %

Fig. S0157a (AIOMFAC_output_0058)

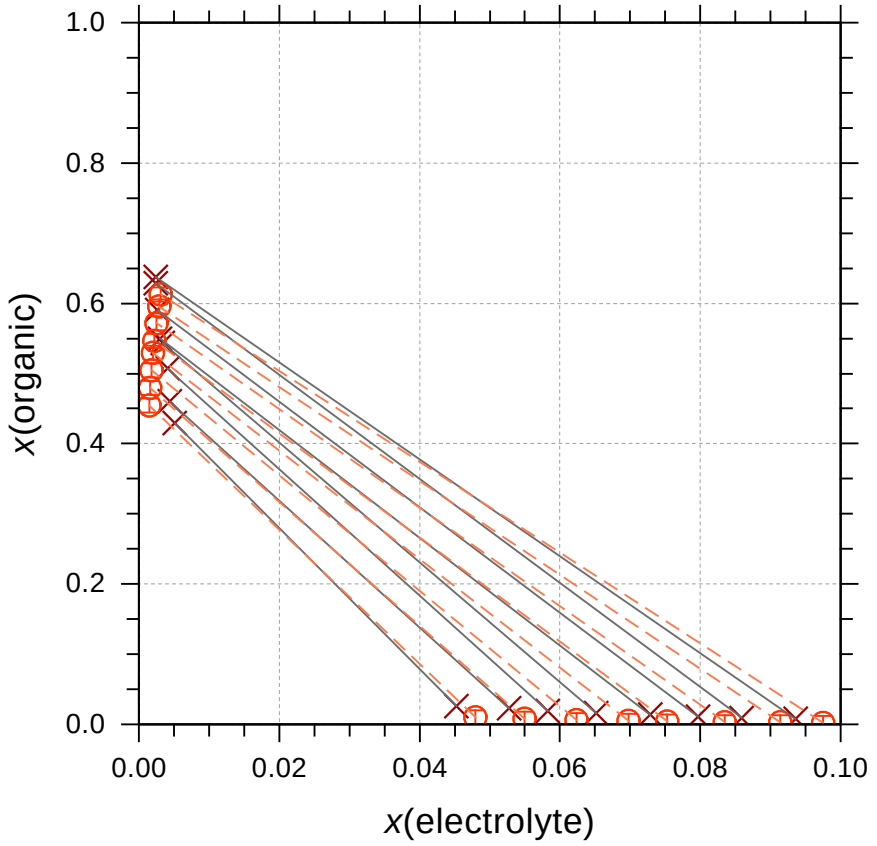
H_2O (1) + *tert*-Butanol (2) + NaCl (3)

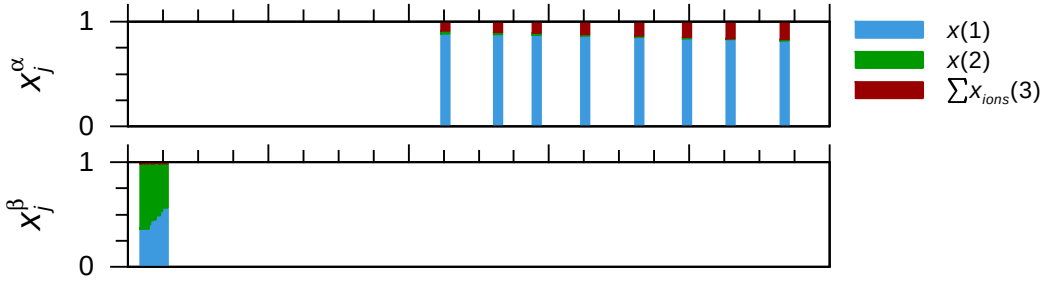
Temperature: 298 K

left y-axis:

× NaCl_tert-BuOH_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0058)$ = 1.000

dataset contribution to F_{obj}:

fval(0058) = 9.8986E-01

rel. contribution = 0.4707 %

Fig. S0158 (AIOMFAC_output_0059)

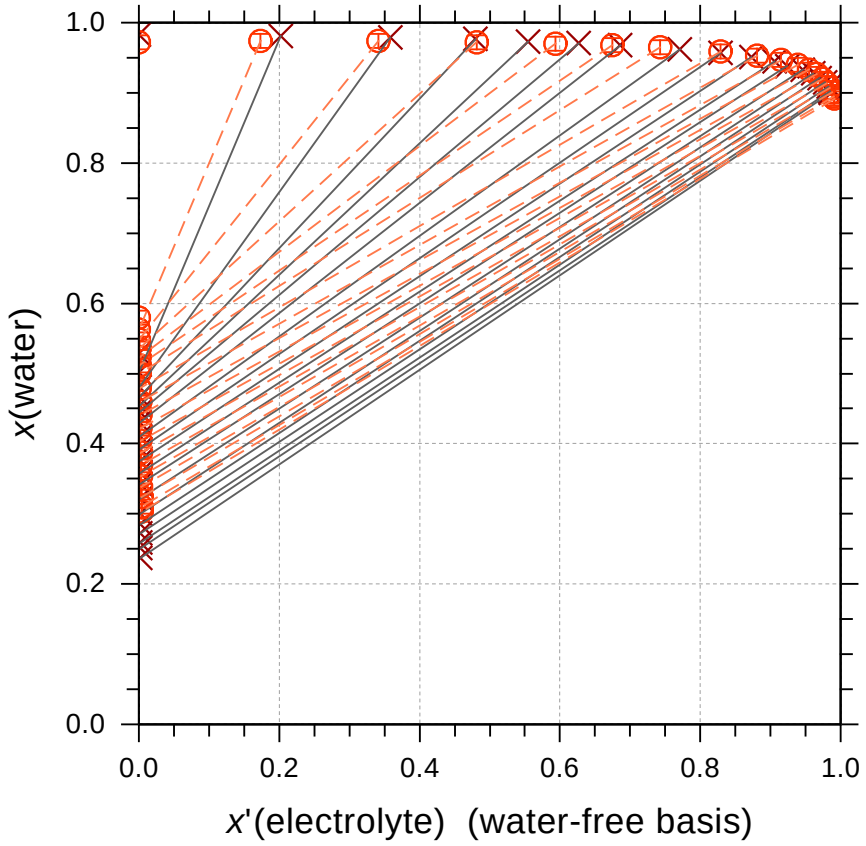
H_2O (1) + 1-Butanol (2) + NaCl (3)

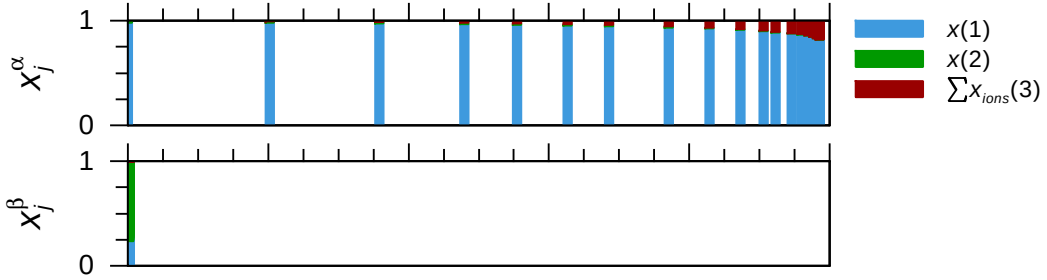
Temperature: 313 K

left y-axis:

× NaCl_1-BuOH_LLE_Santis_40C

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0059) = 0.500

dataset contribution to F_{obj}:

fval(0059) = 3.6016E-02

rel. contribution = 0.0171 %

Fig. S0158a (AIOMFAC_output_0059)

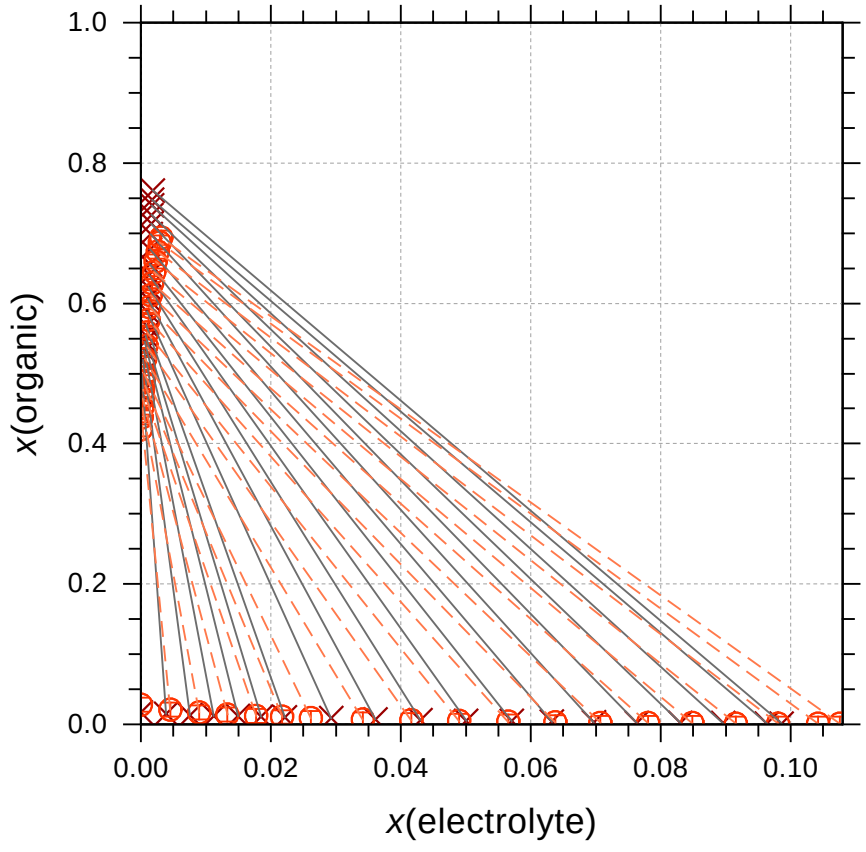
H_2O (1) + 1-Butanol (2) + NaCl (3)

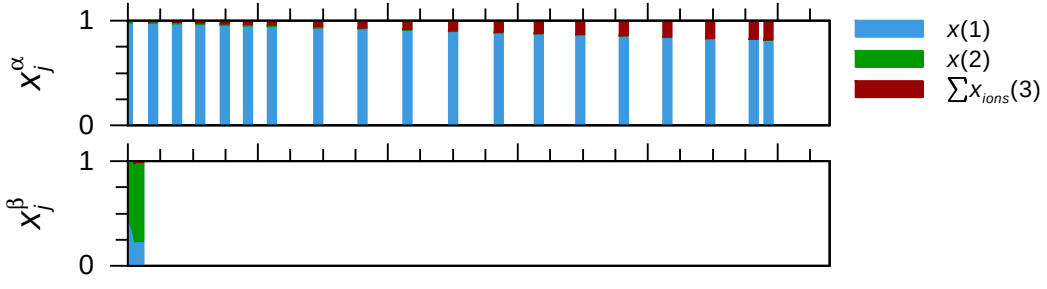
Temperature: 313 K

left y-axis:

× NaCl_1-BuOH_LLE_Santis_40C

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0059) = 0.500

dataset contribution to F_{obj}:

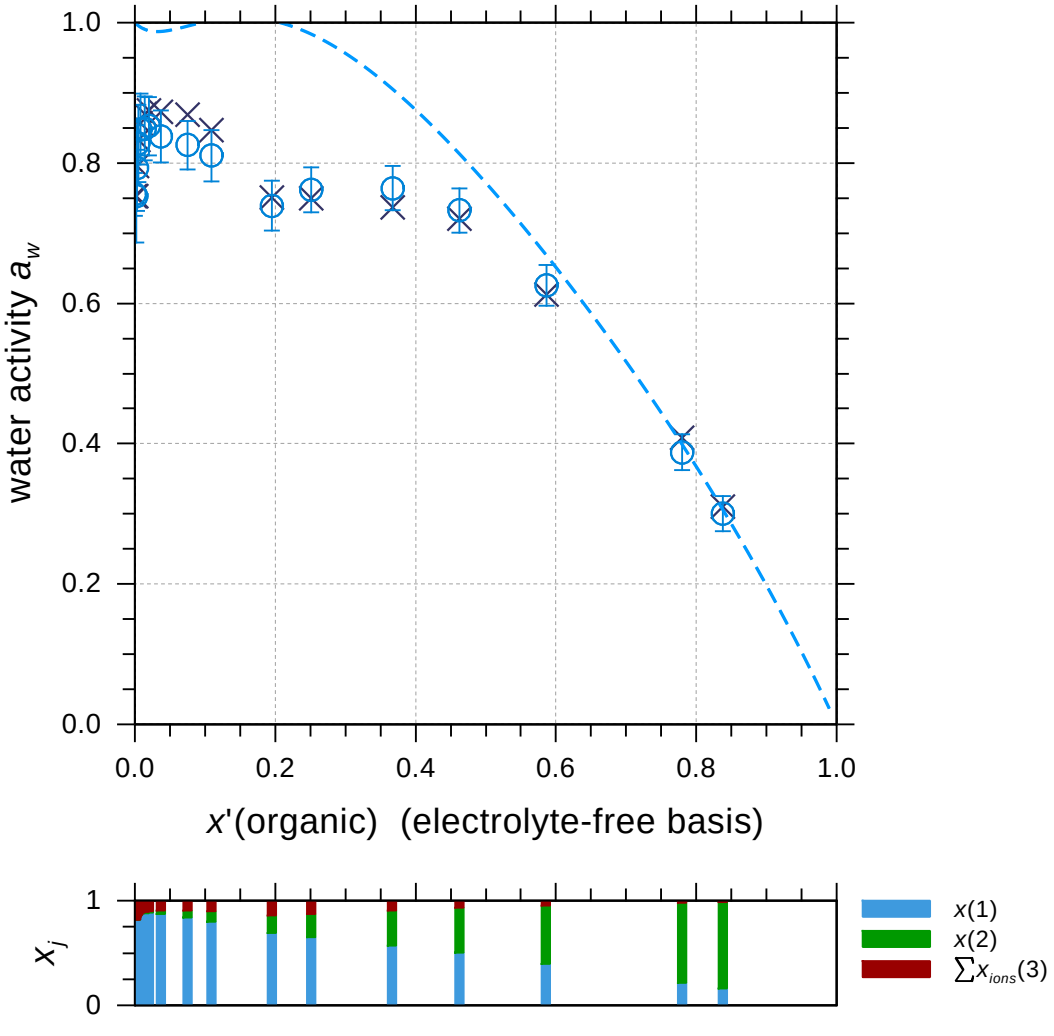
fval(0059) = 3.6016E-02

rel. contribution = 0.0171 %

Fig. S0159 (AIOMFAC_output_0060)

H_2O (1) + 1,2-Hexanediol (2) + NaCl (3)

Temperature: 298 K

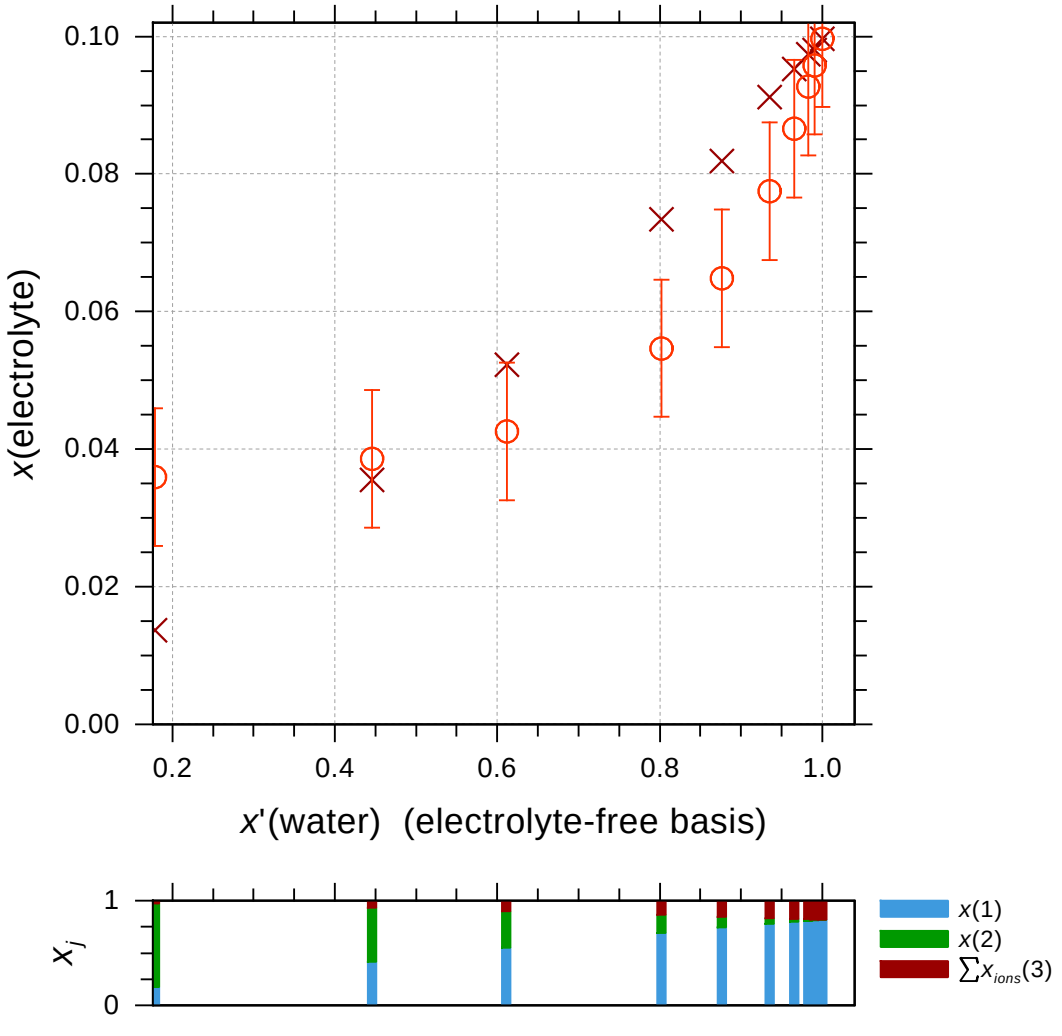


initial weighting of dataset:
$w^{init}(0060)$ = 2.000
dataset contribution to F_{obj}:
fval(0060) = 1.4252E-02
rel. contribution = 0.0068 %

Fig. S0160 (AIOMFAC_output_0952)

H_2O (1) + Glycerol (2) + NaCl (3)

Temperature: 298 K

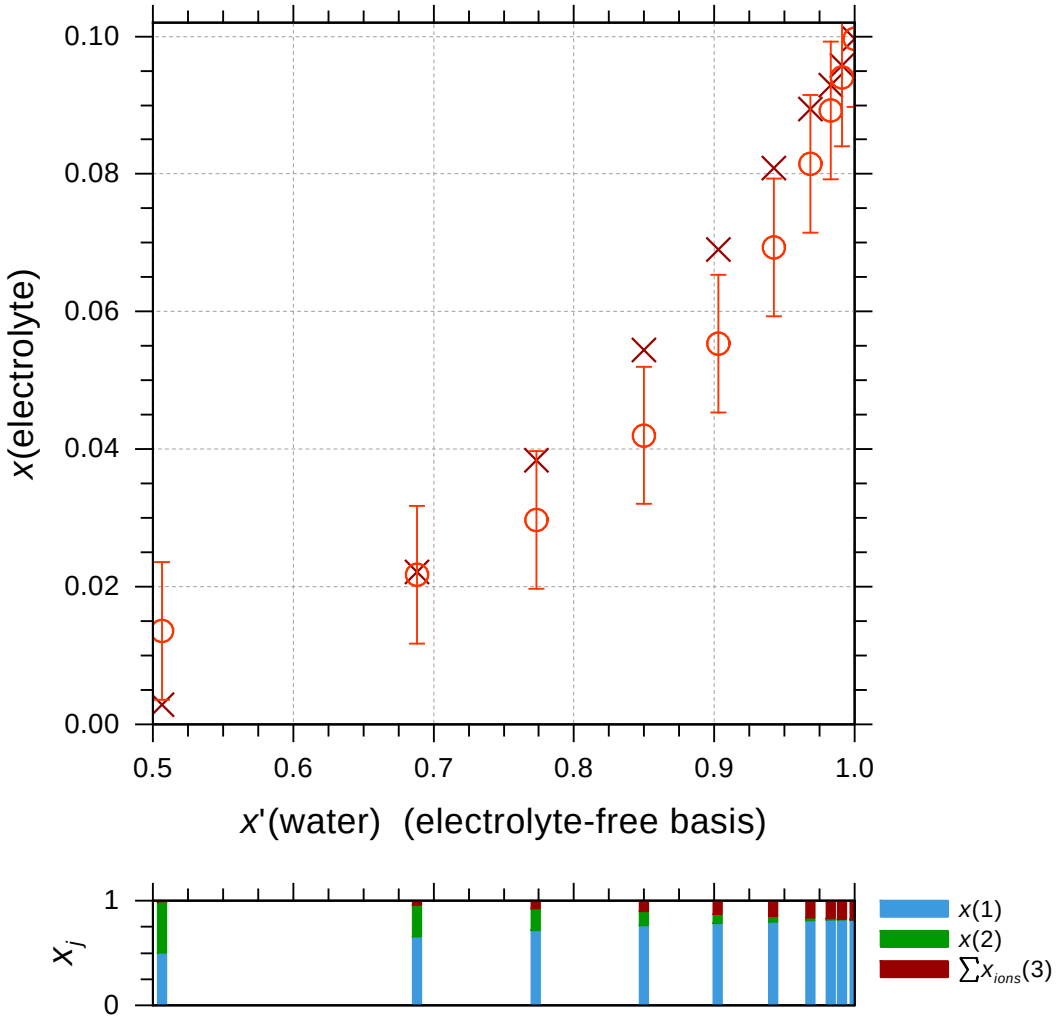


initial weighting of dataset:
w^{init}(0952) = 1.000
dataset contribution to F_{obj}:
fval(0952) = 1.0350E+00
rel. contribution = 0.4922 %

Fig. S0161 (AIOMFAC_output_0953)

H_2O (1) + 1,4-Butanediol (2) + NaCl (3)

Temperature: 298 K

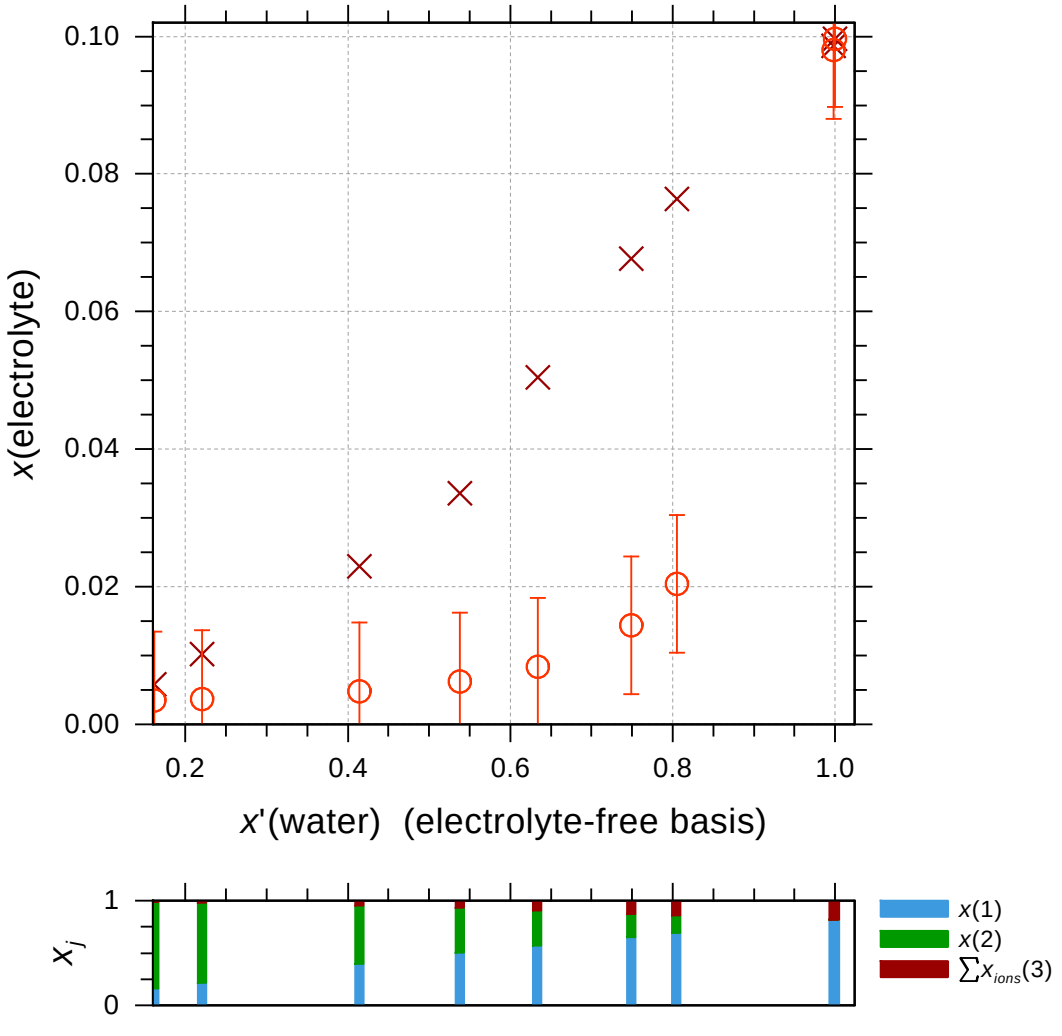


initial weighting of dataset:
$w^{init}(0953)$ = 1.000
dataset contribution to F_{obj}:
fval(0953) = 8.2885E-01
rel. contribution = 0.3941 %

Fig. S0162 (AIOMFAC_output_0954)

H_2O (1) + 1,2-Hexanediol (2) + NaCl (3)

Temperature: 298 K

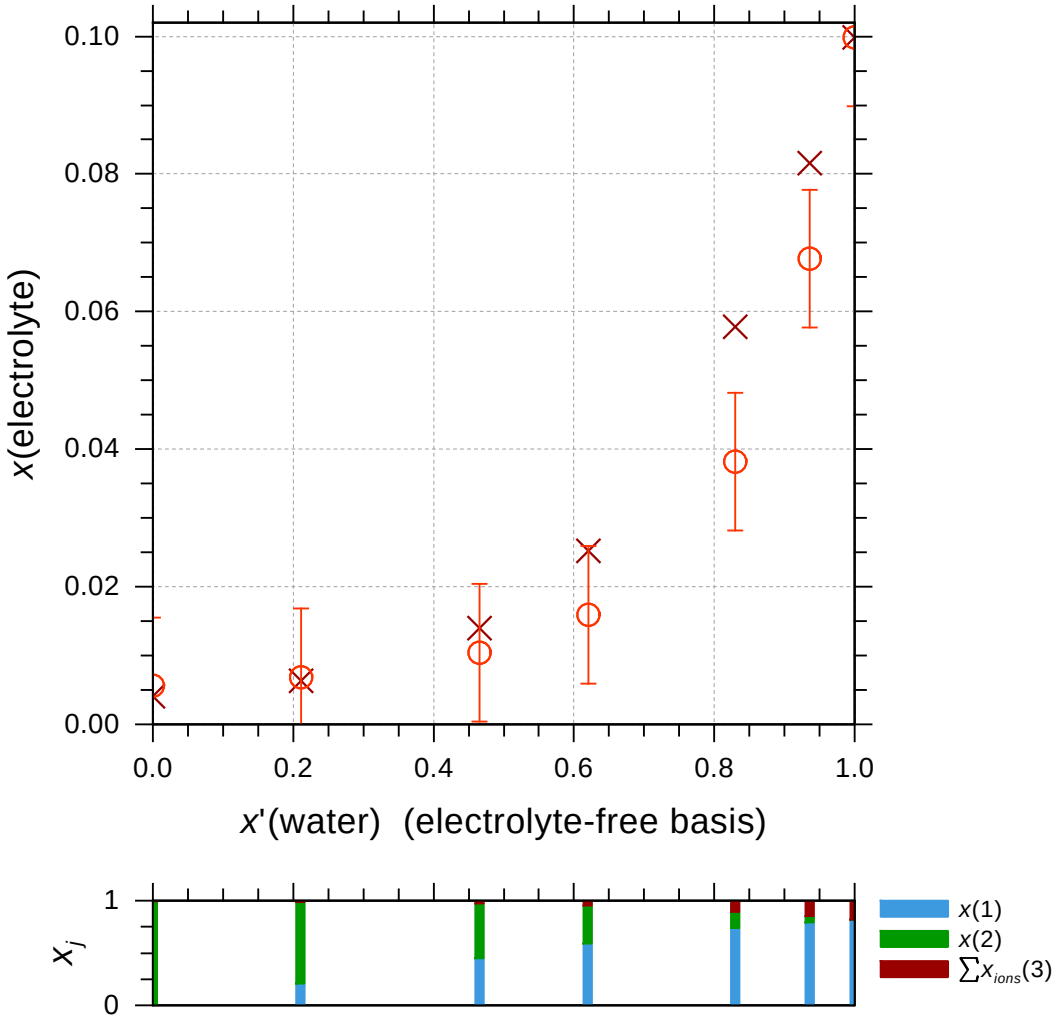


initial weighting of dataset:
$w^{init}(0954)$ = 1.000
dataset contribution to F_{obj}:
fval(0954) = 2.2178E+00
rel. contribution = 1.0546 %

Fig. S0163 (AIOMFAC_output_0400)

H_2O (1) + 1,4-Dihydroxy-2-butene (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:
w^{init}(0400) = 1.000
dataset contribution to F_{obj}:
fval(0400) = 2.1349E-01
rel. contribution = 0.1015 %

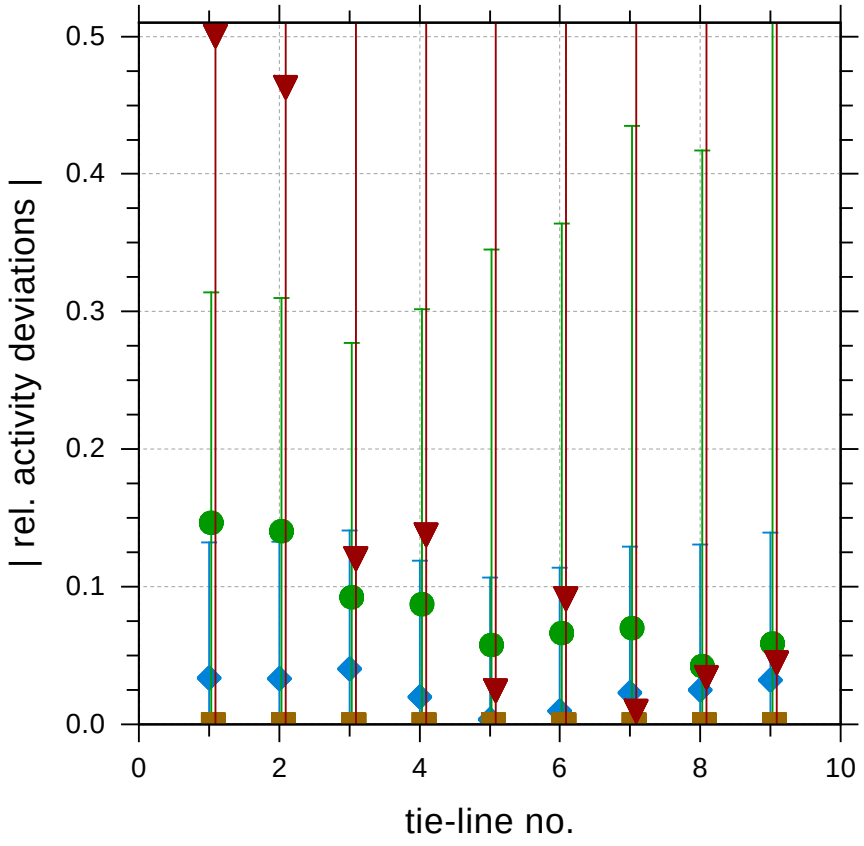
Fig. S0164 (AIOMFAC_output_1008)

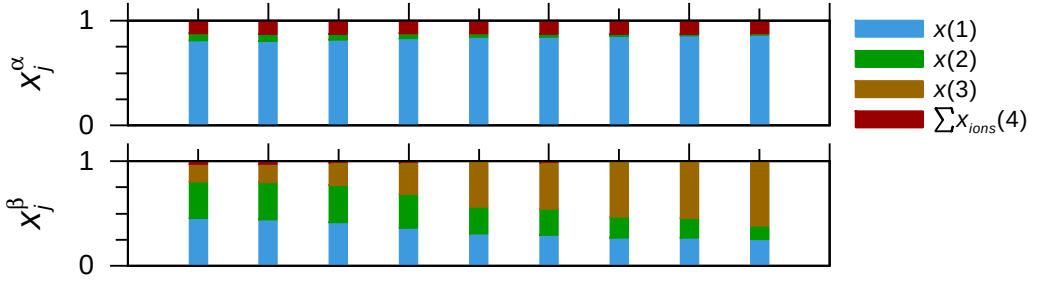
H_2O (1) + Ethanol (2) + 3-Methyl-1-butanol (3) + NaCl (4)

Temperature: 298 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



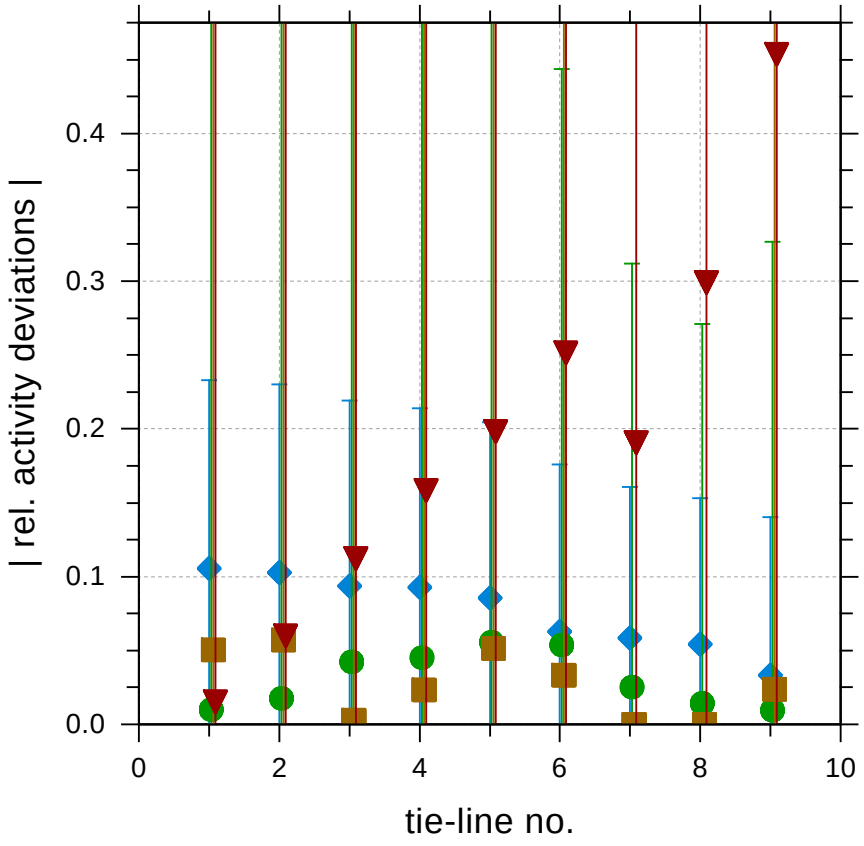


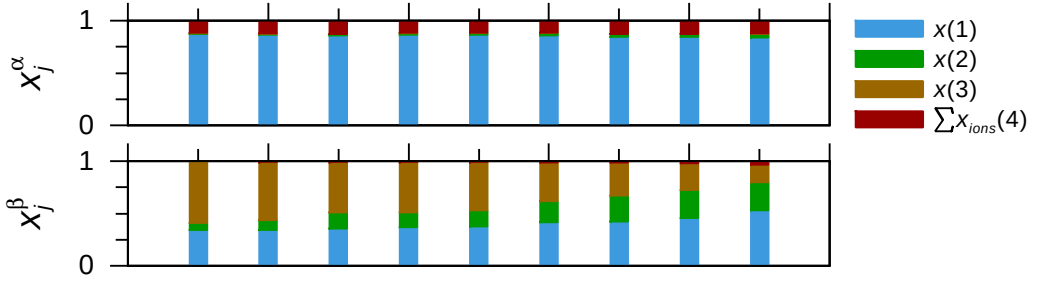
initial weighting of dataset:
$w^{init}(1008)$ = 1.000
dataset contribution to F_{obj}:
fval(1008) = 3.2901E-01
rel. contribution = 0.1565 %

Fig. S0165 (AIOMFAC_output_1011)

H_2O (1) + Ethanol (2) + 1-Butanol (3) + NaCl (4)

Temperature: 298 K



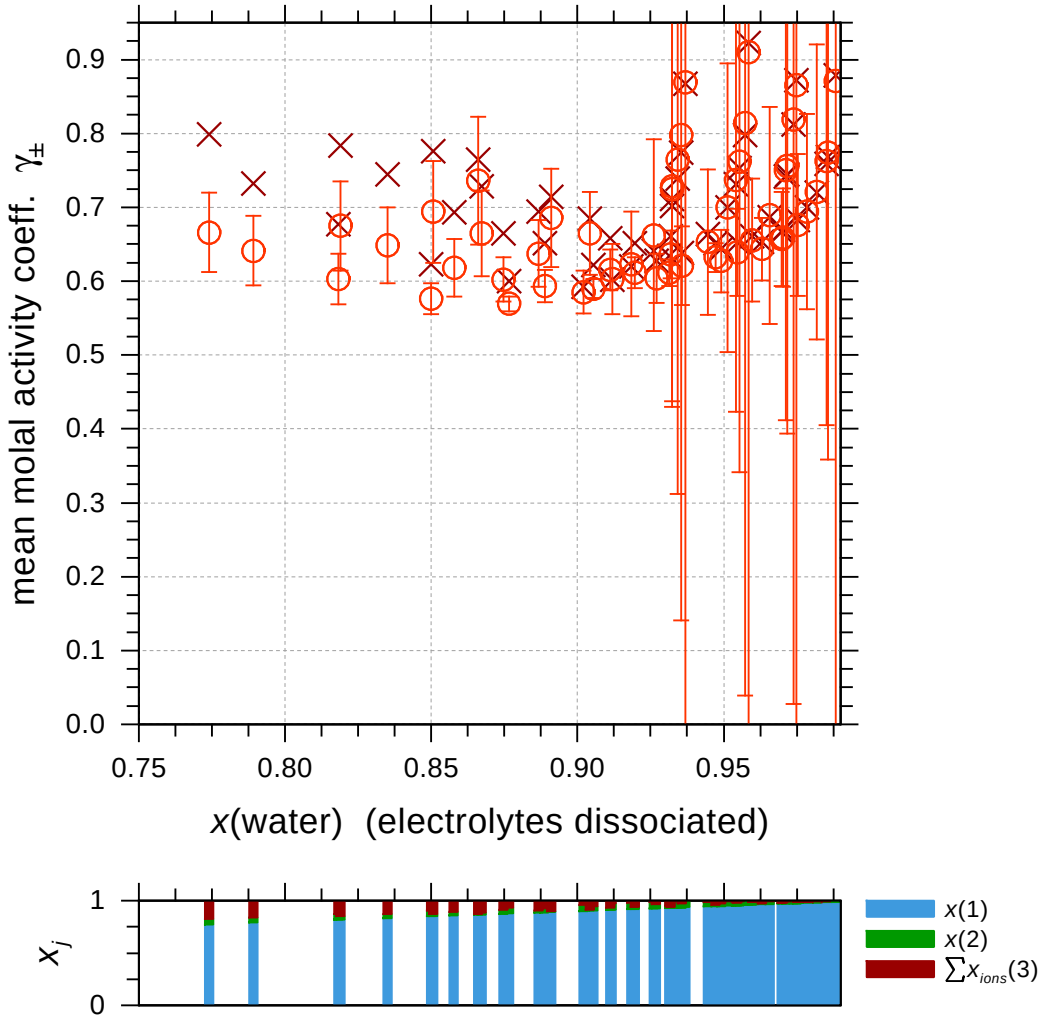


initial weighting of dataset:
$w^{init}(1011)$ = 1.000
dataset contribution to F_{obj}:
fval(1011) = 3.0850E-01
rel. contribution = 0.1467 %

Fig. S0166 (AIOMFAC_output_1029)

H_2O (1) + D-Fructopyranose (2) + NaCl (3)

Temperature: 298 K

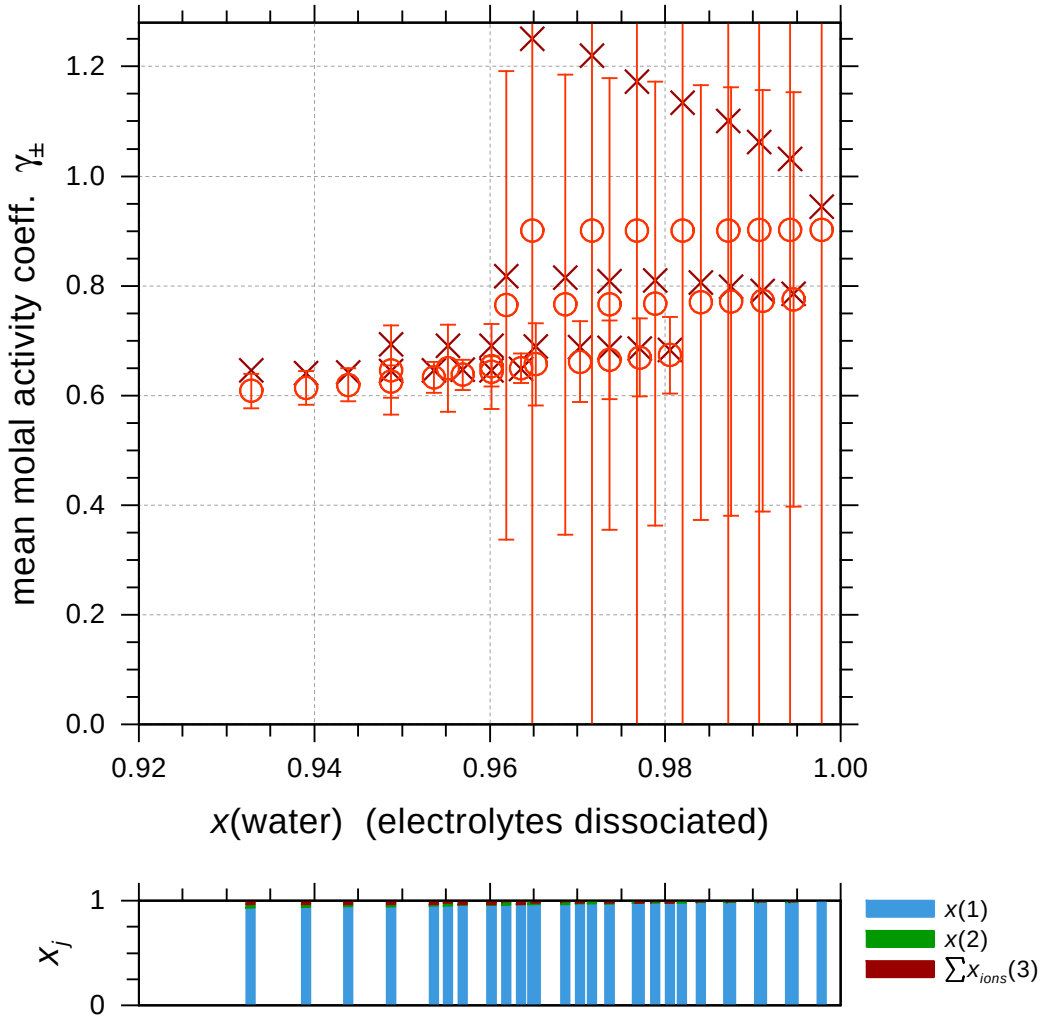


initial weighting of dataset:
$w^{init}(1029)$ = 2.000
dataset contribution to F_{obj}:
fval(1029) = 5.6728E-02
rel. contribution = 0.0270 %

Fig. S0167 (AIOMFAC_output_1041)

H_2O (1) + D-Mannopyranose (2) + NaCl (3)

Temperature: 298 K

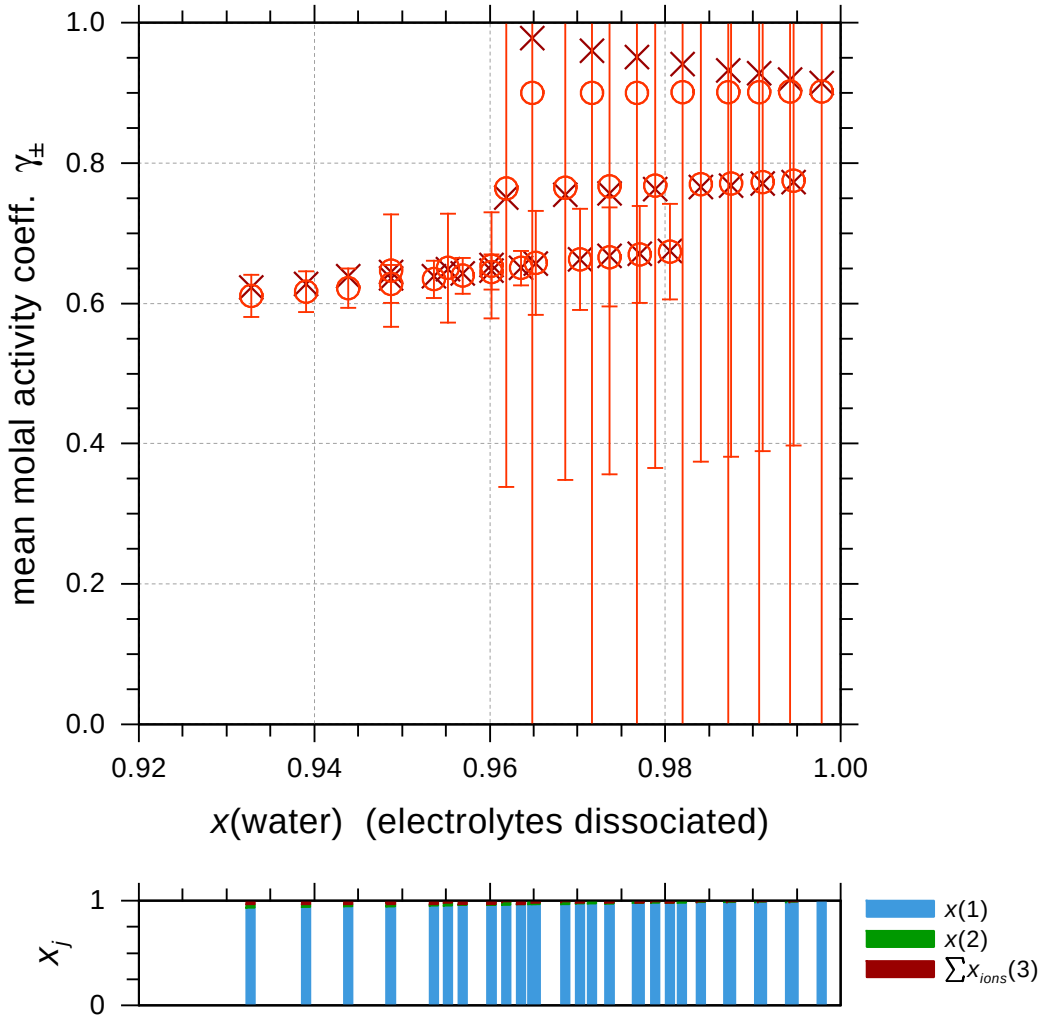


initial weighting of dataset:
$w^{init}(1041)$ = 2.000
dataset contribution to F_{obj}:
fval(1041) = 3.9260E-02
rel. contribution = 0.0187 %

Fig. S0168 (AIOMFAC_output_1044)

H_2O (1) + D-Ribofuranose (2) + NaCl (3)

Temperature: 298 K

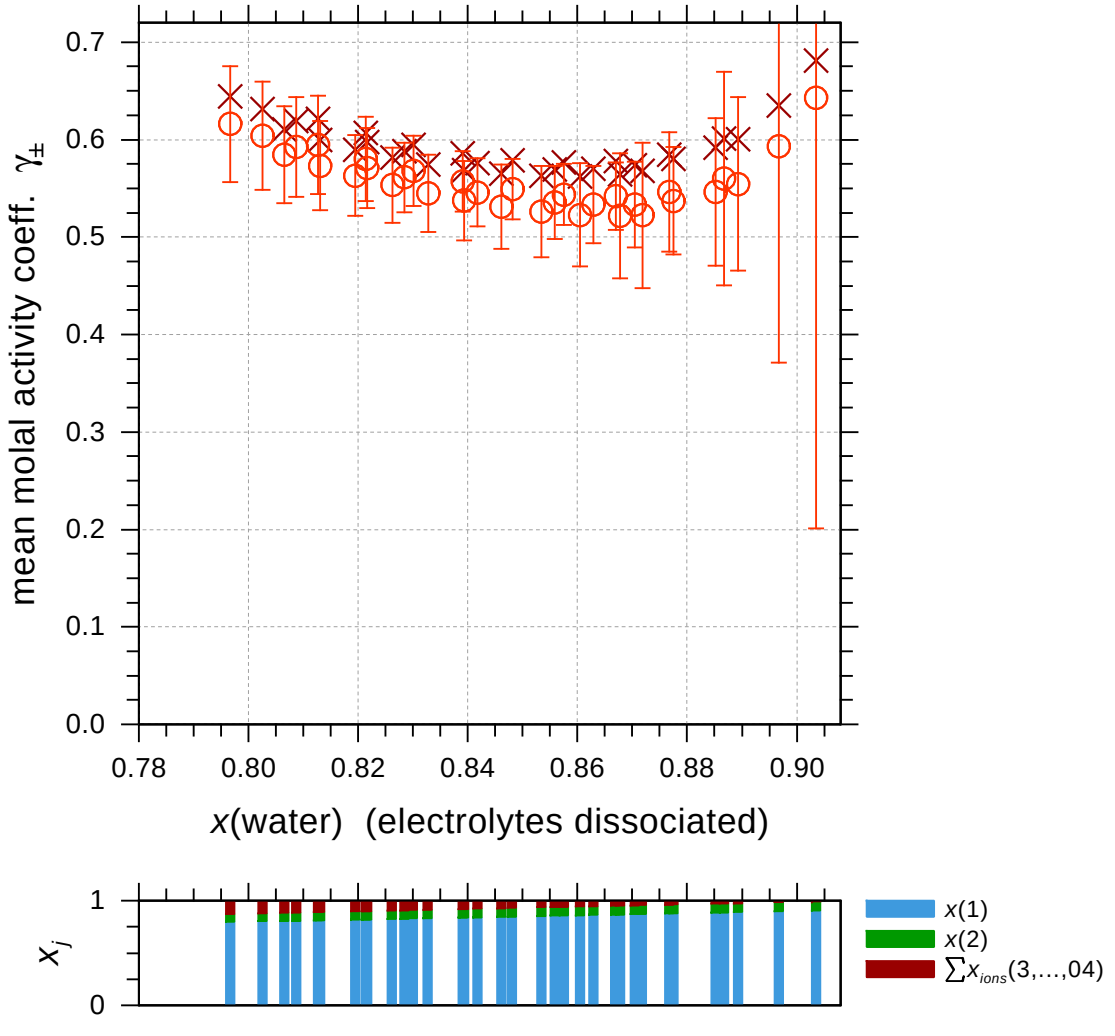


initial weighting of dataset:
$w^{init}(1044)$ = 2.000
dataset contribution to F_{obj}:
fval(1044) = 1.9795E-03
rel. contribution = 0.0009 %

Fig. S0169 (AIOMFAC_output_0111)

H_2O (1) + Ethanol (2) + NaCl (3) + KCl (4)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0111)$ = 2.000

dataset contribution to F_{obj}:

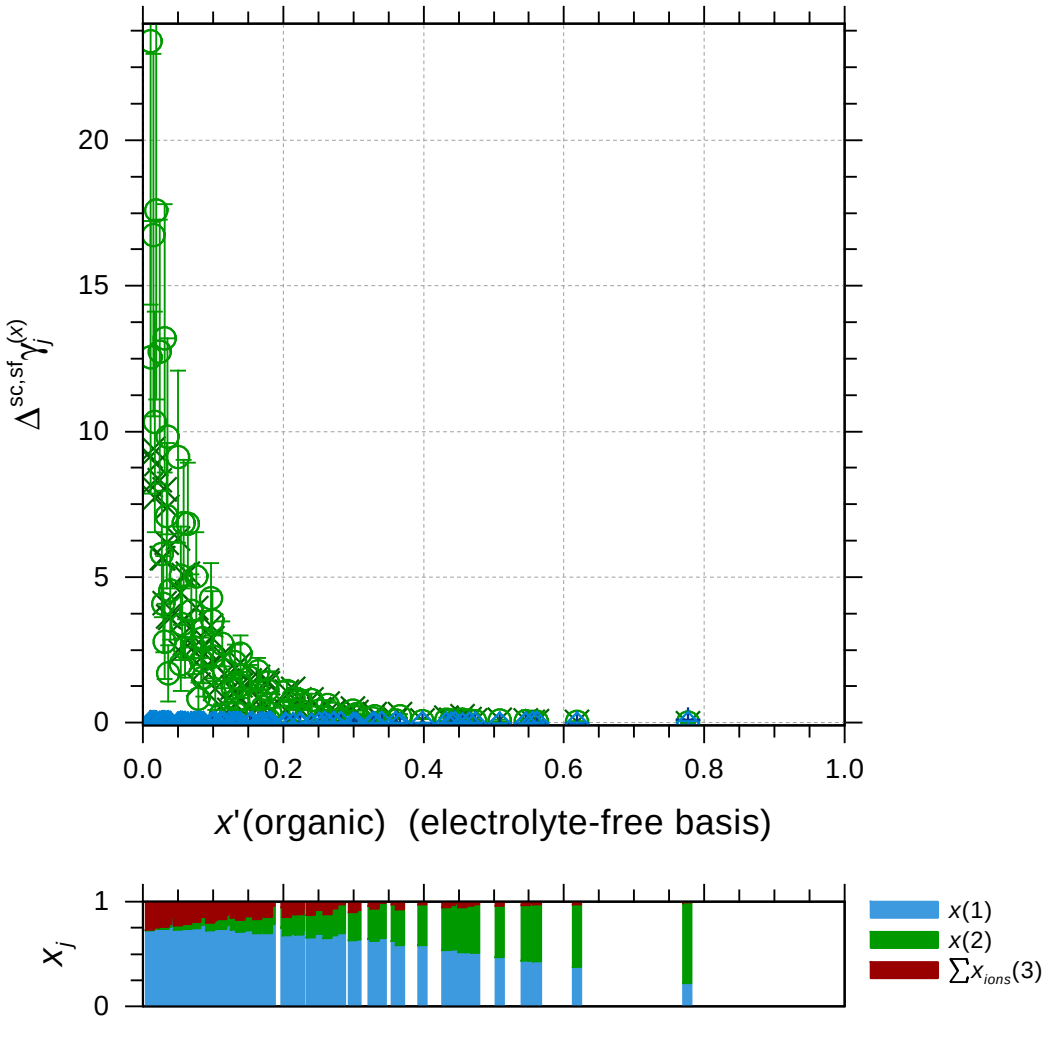
fval(0111) = 1.2781E-01

rel. contribution = 0.0608 %

Fig. S0170 (AIOMFAC_output_0067)

H_2O (1) + Ethanol (2) + $NaNO_3$ (3)

Temperature range: 351 -- 374 K

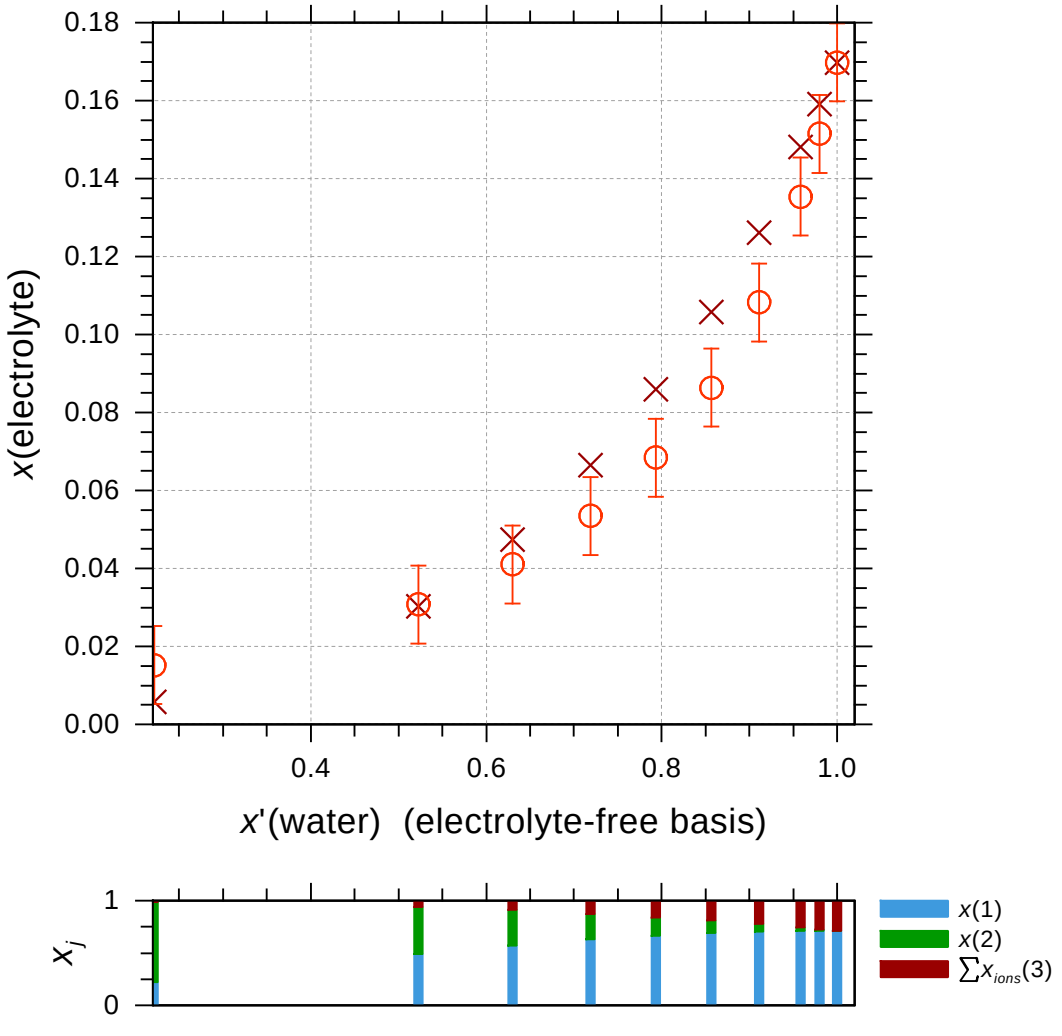


initial weighting of dataset:
w^{init}(0067) = 0.500
dataset contribution to F_{obj}:
fval(0067) = 1.3403E-01
rel. contribution = 0.0637 %

Fig. S0171 (AIOMFAC_output_0068)

H_2O (1) + Ethanol (2) + $NaNO_3$ (3)

Temperature: 303 K

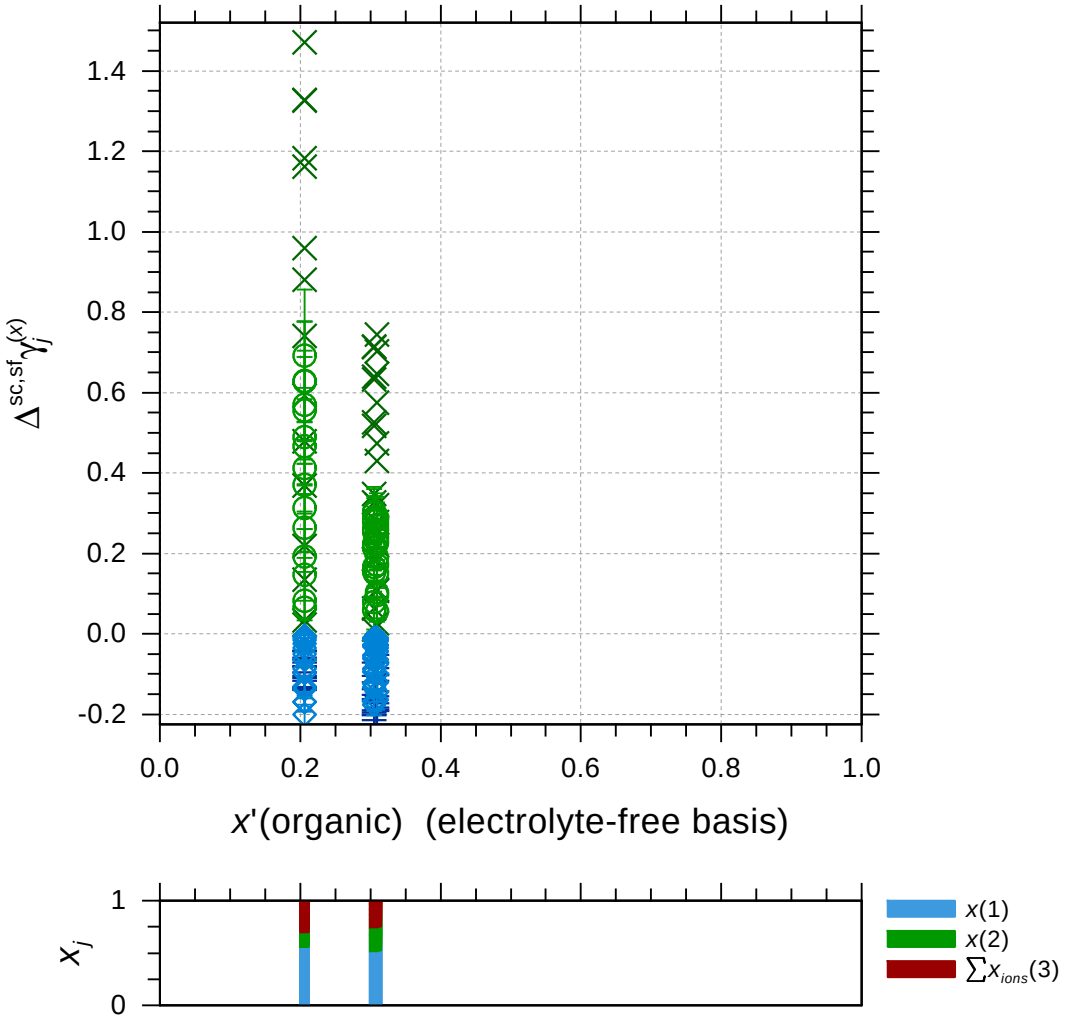


initial weighting of dataset:
w^{init}(0068) = 0.500
dataset contribution to F_{obj}:
fval(0068) = 2.4764E-01
rel. contribution = 0.1178 %

Fig. S0172 (AIOMFAC_output_0109)

H_2O (1) + Ethanol (2) + NH_4Br (3)

Temperature range: 356 -- 359 K

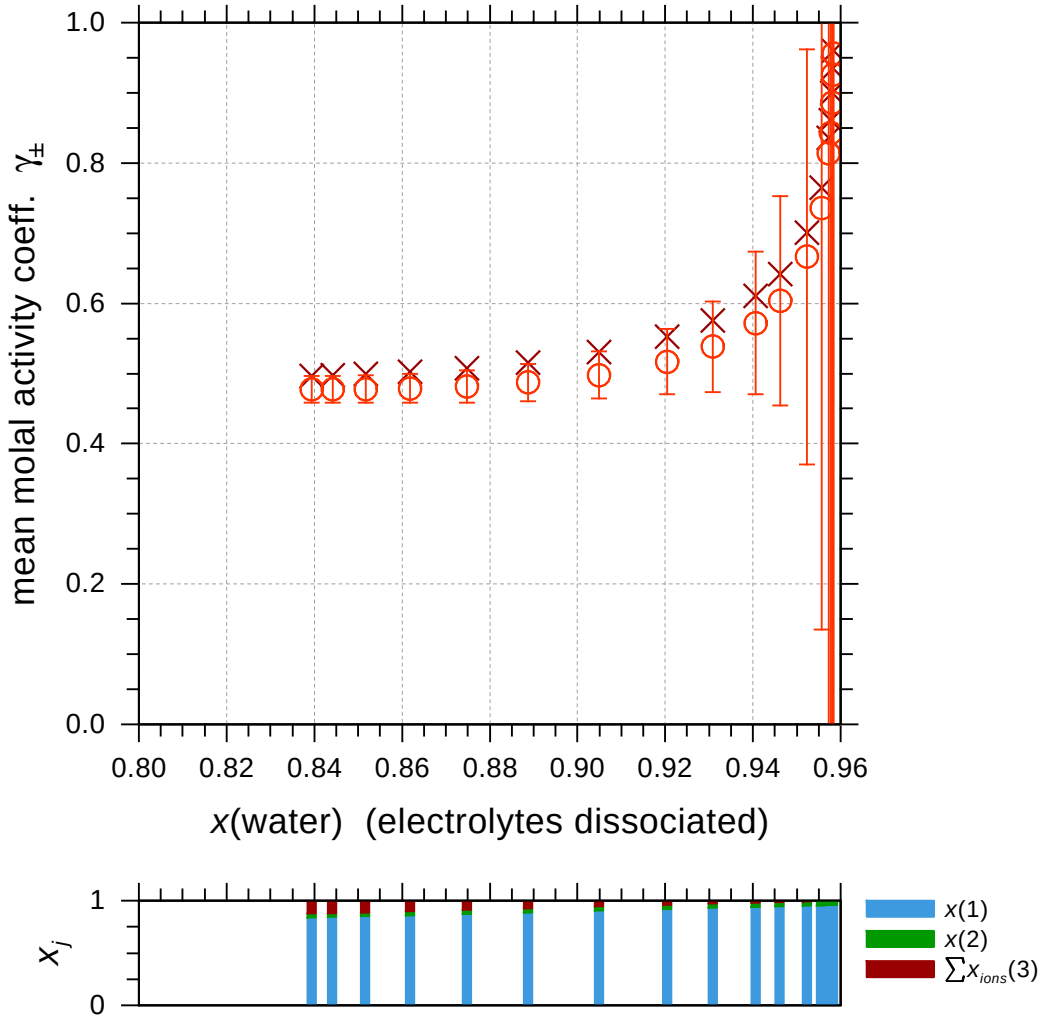


initial weighting of dataset:
$w^{init}(0109)$ = 0.500
dataset contribution to F_{obj}:
fval(0109) = 1.5467E-01
rel. contribution = 0.0736 %

Fig. S0173 (AIOMFAC_output_0001)

H_2O (1) + Ethanol (2) + NH_4Cl (3)

Temperature: 298 K

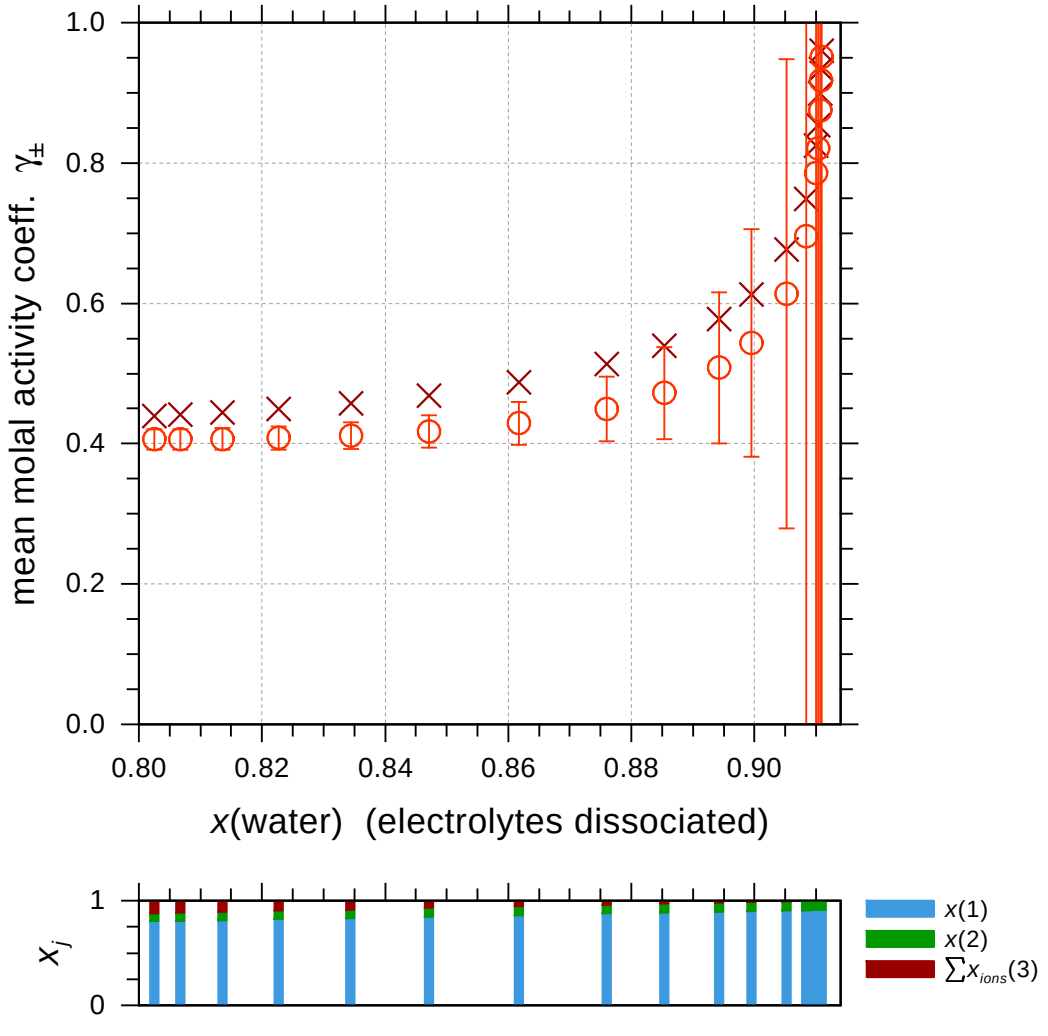


initial weighting of dataset:
$w^{init}(0001)$ = 2.000
dataset contribution to F_{obj}:
fval(0001) = 3.2218E-02
rel. contribution = 0.0153 %

Fig. S0174 (AIOMFAC_output_0002)

H_2O (1) + Ethanol (2) + NH_4Cl (3)

Temperature: 298 K

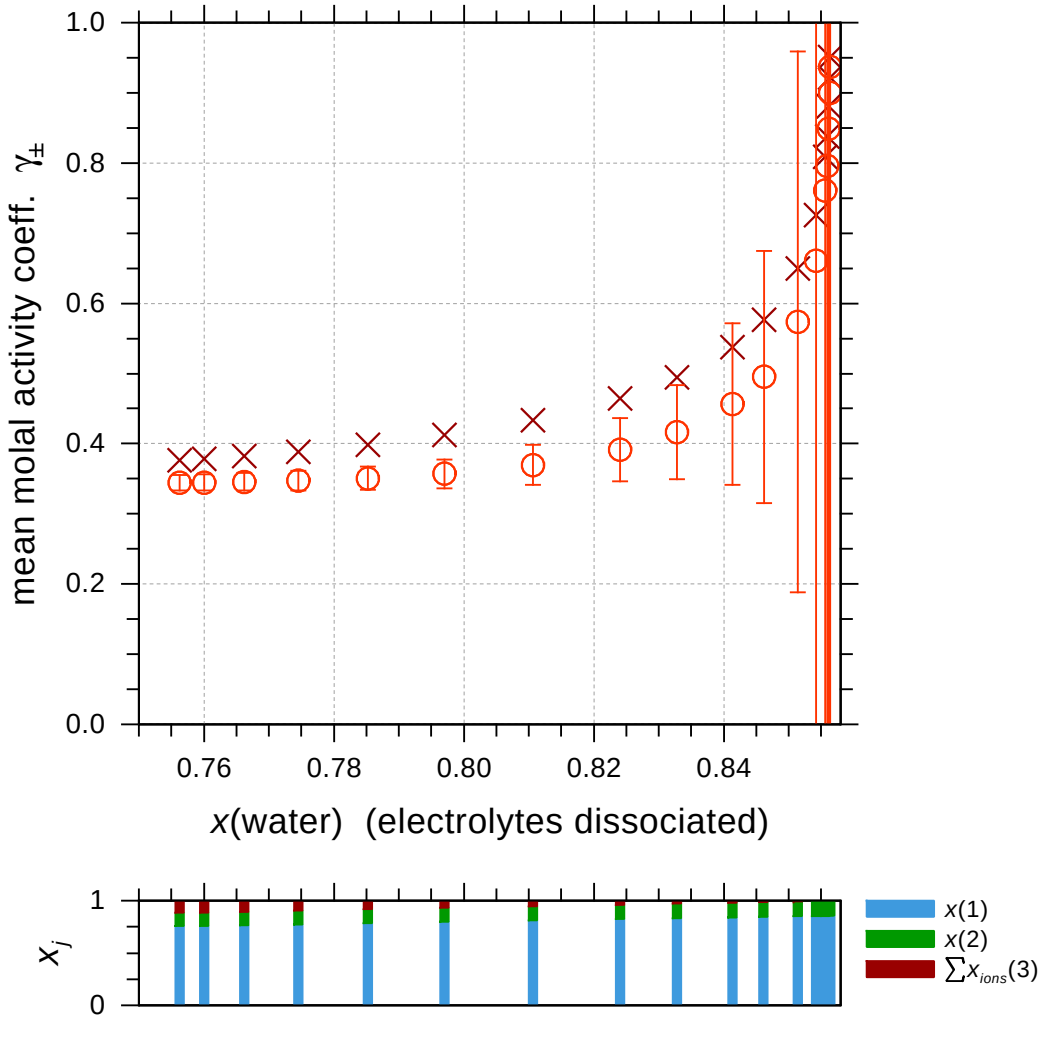


initial weighting of dataset:
$w^{init}(0002)$ = 2.000
dataset contribution to F_{obj}:
fval(0002) = 1.2096E-01
rel. contribution = 0.0575 %

Fig. S0175 (AIOMFAC_output_0003)

H_2O (1) + Ethanol (2) + NH_4Cl (3)

Temperature: 298 K

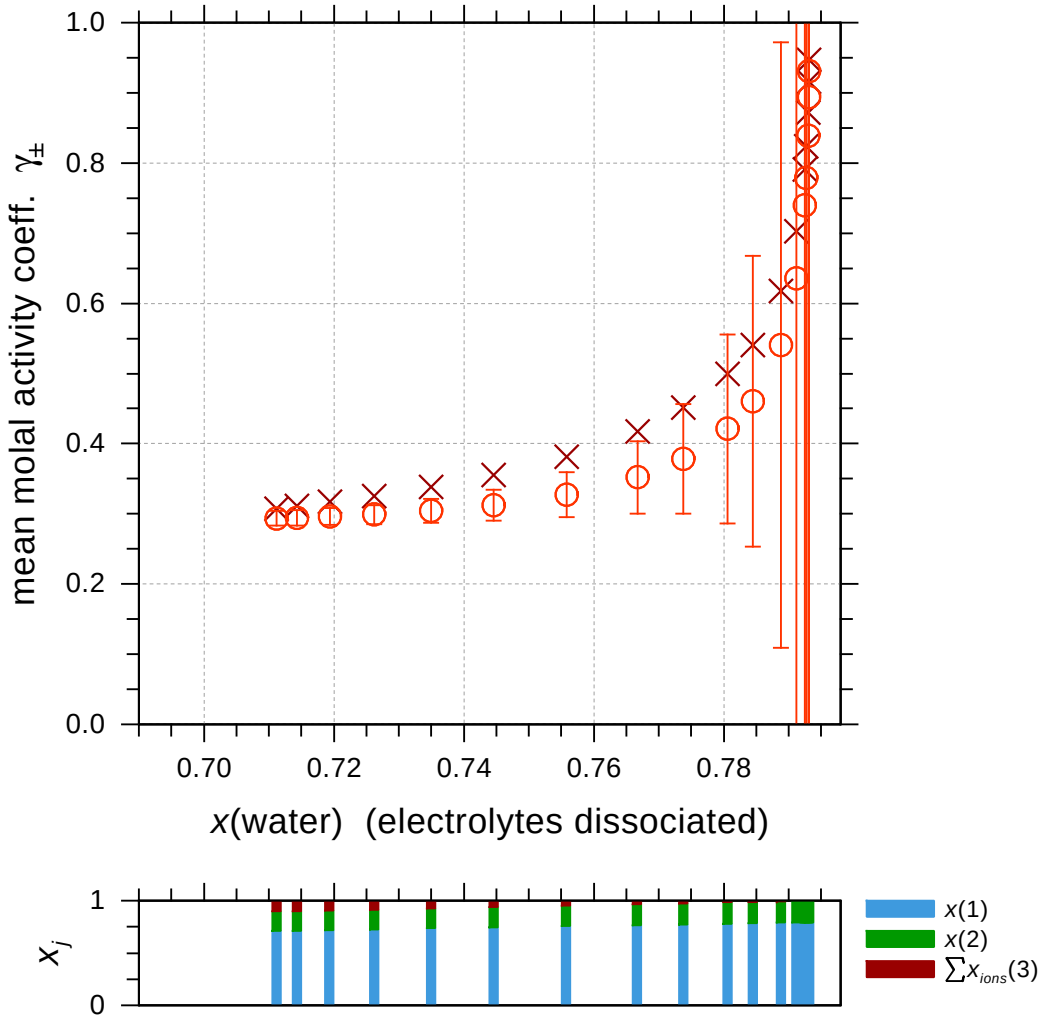


initial weighting of dataset:
$w^{init}(0003)$ = 2.000
dataset contribution to F_{obj}:
fval(0003) = 1.7365E-01
rel. contribution = 0.0826 %

Fig. S0176 (AIOMFAC_output_0004)

H_2O (1) + Ethanol (2) + NH_4Cl (3)

Temperature: 298 K

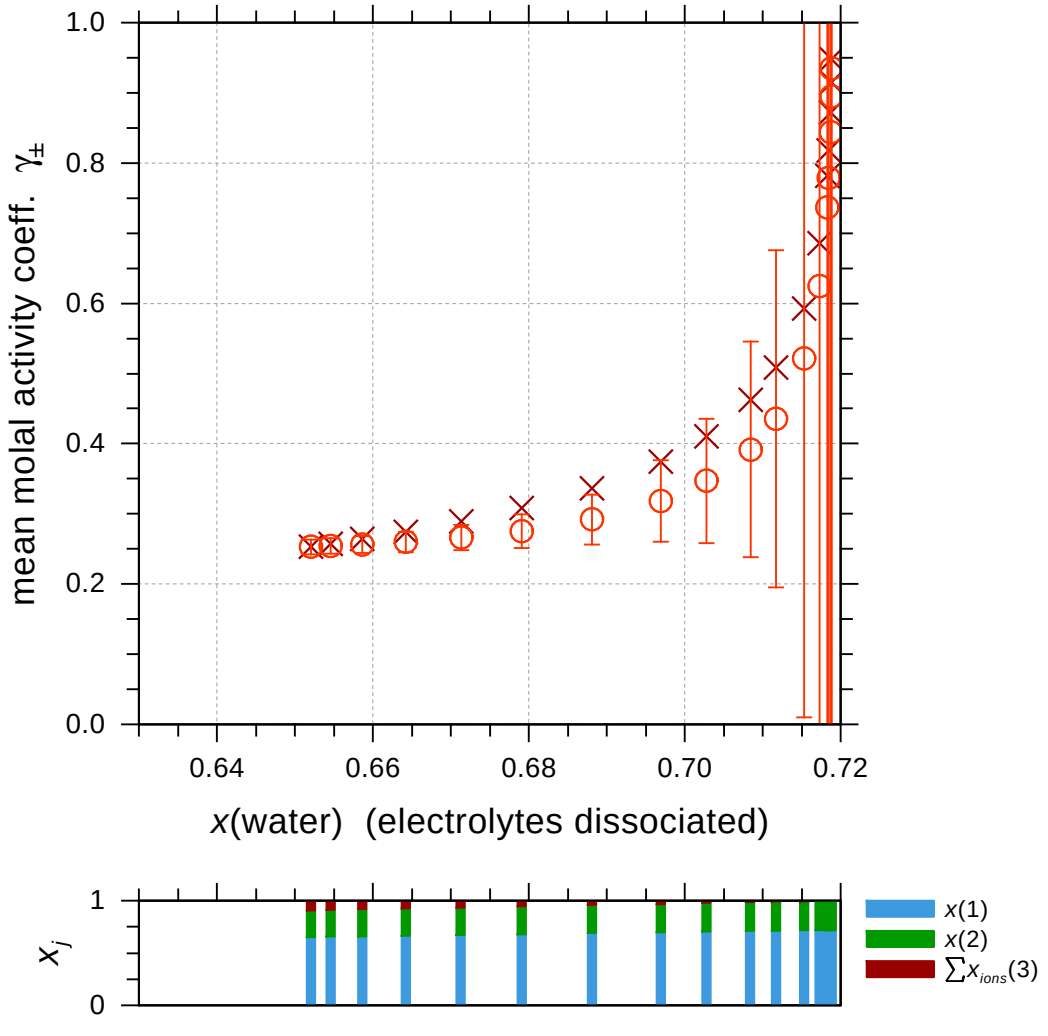


initial weighting of dataset:
$w^{init}(0004)$ = 2.000
dataset contribution to F_{obj}:
fval(0004) = 1.4242E-01
rel. contribution = 0.0677 %

Fig. S0177 (AIOMFAC_output_0005)

H_2O (1) + Ethanol (2) + NH_4Cl (3)

Temperature: 298 K

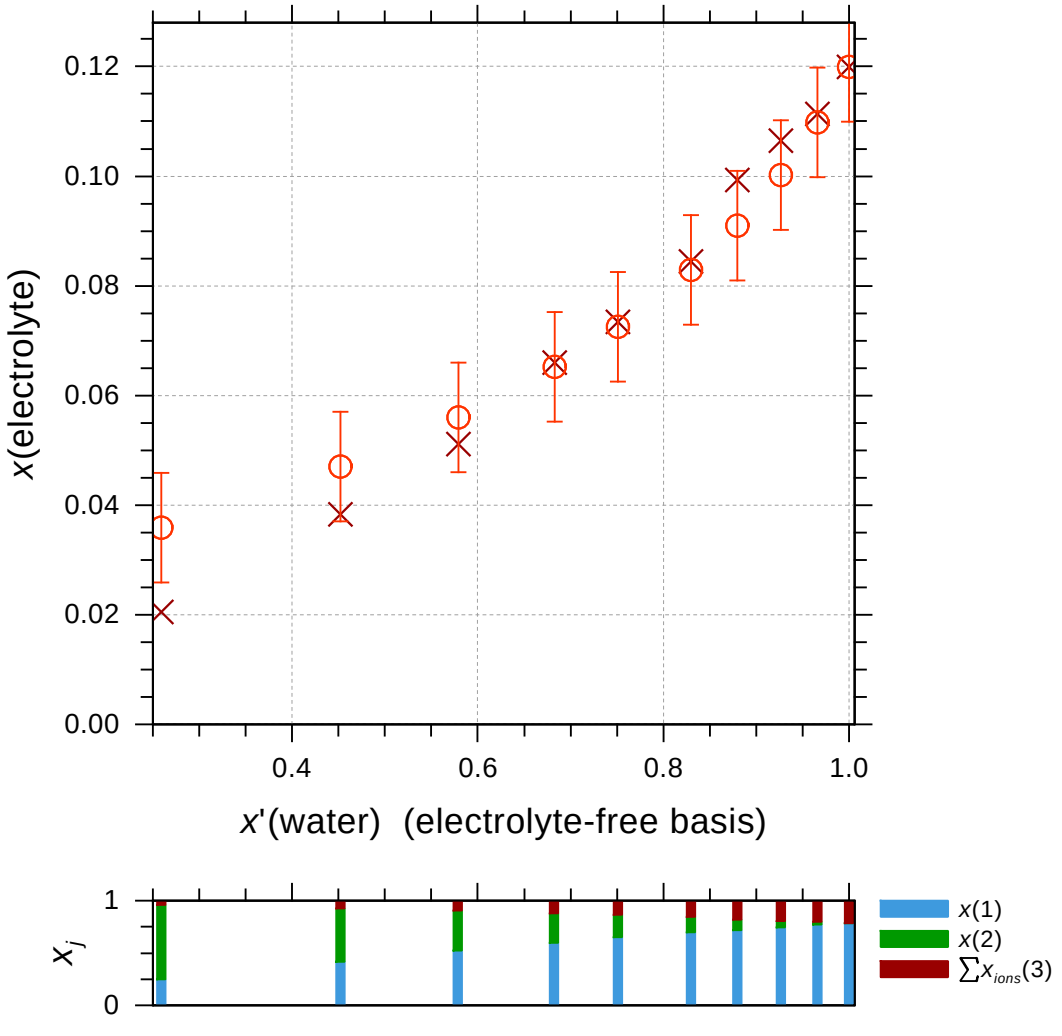


initial weighting of dataset:
$w^{init}(0005)$ = 2.000
dataset contribution to F_{obj}:
fval(0005) = 1.0429E-01
rel. contribution = 0.0496 %

Fig. S0178 (AIOMFAC_output_0006)

H_2O (1) + Ethanol (2) + NH_4Cl (3)

Temperature: 303 K

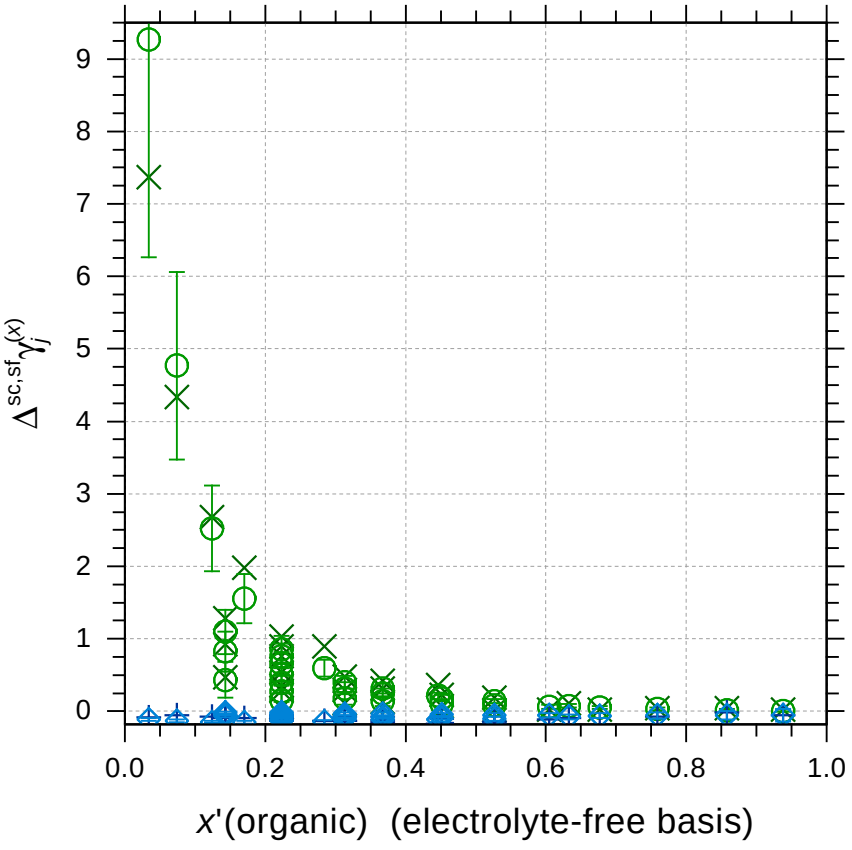


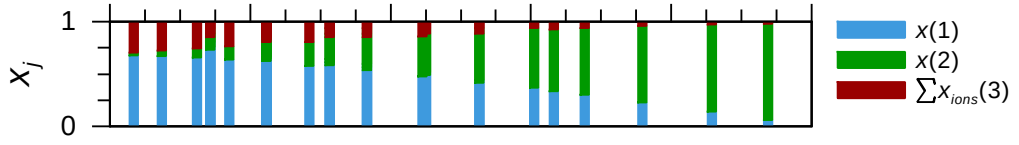
initial weighting of dataset:
w^{init}(0006) = 1.000
dataset contribution to F_{obj}:
fval(0006) = 3.0501E-01
rel. contribution = 0.1450 %

Fig. S0179 (AIOMFAC_output_0007)

H_2O (1) + Ethanol (2) + NH_4Cl (3)

Temperature range: 351 -- 367 K



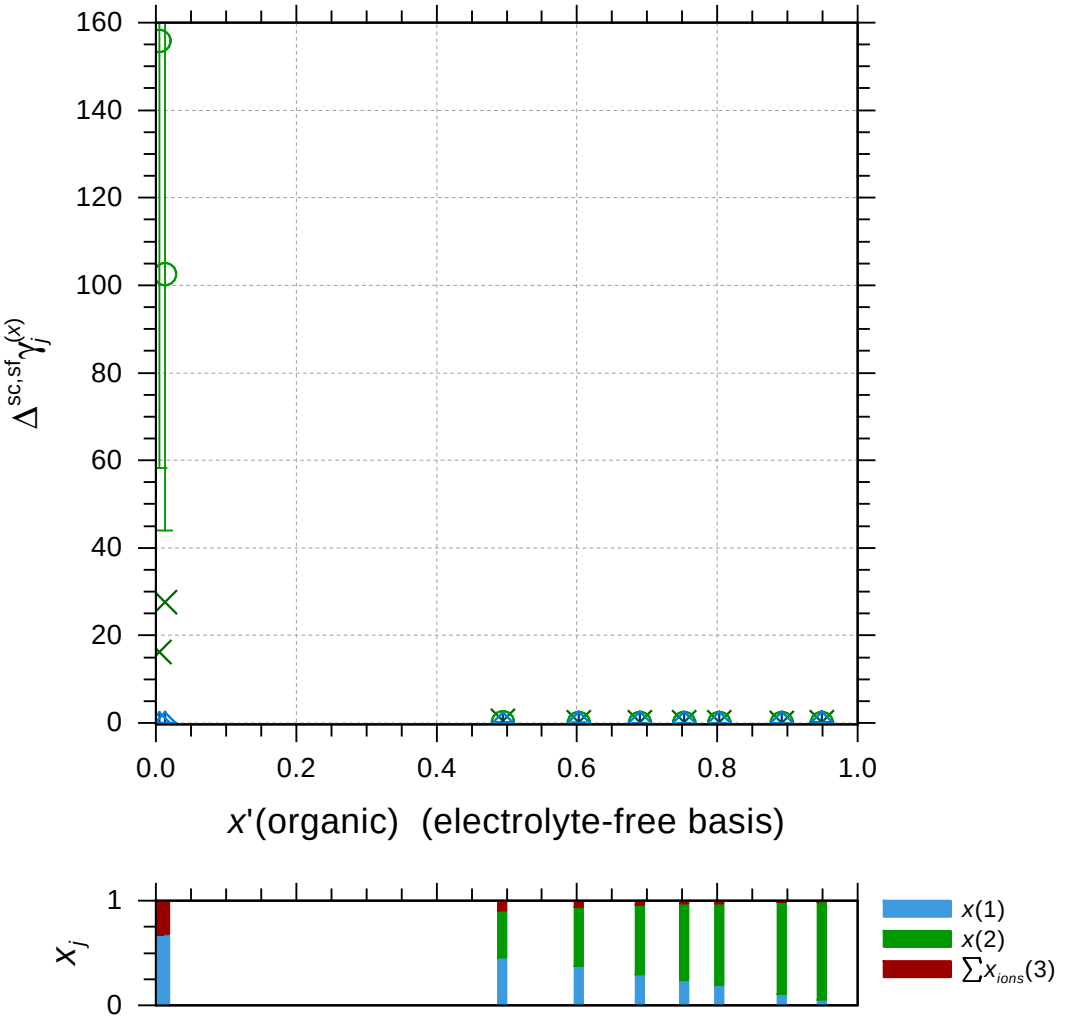


initial weighting of dataset:
$w^{init}(0007)$ = 0.500
dataset contribution to F_{obj}:
fval(0007) = 3.1296E-02
rel. contribution = 0.0149 %

Fig. S0180 (AIOMFAC_output_0027)

H_2O (1) + 1-Propanol (2) + NH_4Cl (3)

Temperature range: 363 -- 384 K

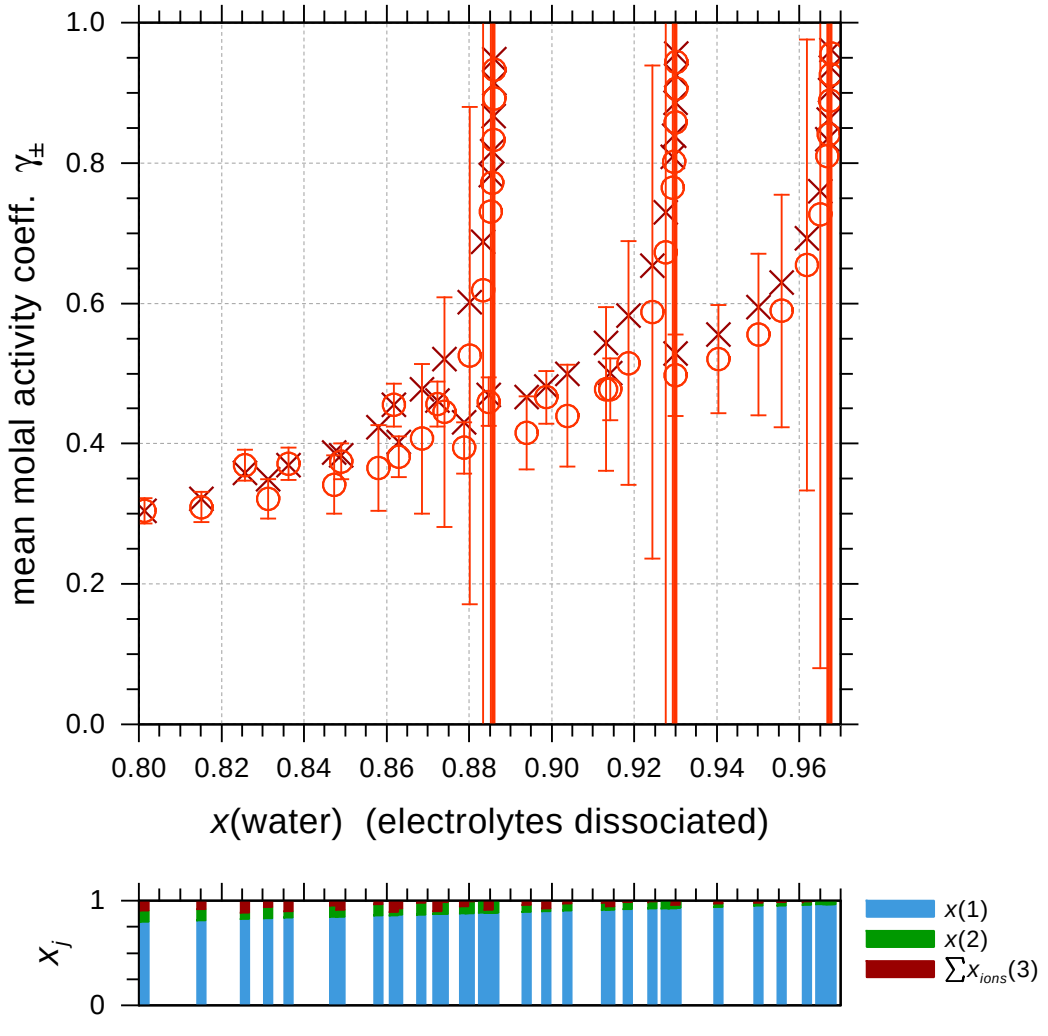


initial weighting of dataset:
$w^{init}(0027)$ = 0.500
dataset contribution to F_{obj}:
fval(0027) = 1.2430E+00
rel. contribution = 0.5911 %

Fig. S0181 (AIOMFAC_output_1047)

H_2O (1) + 2-Propanol (2) + NH_4Cl (3)

Temperature: 298 K

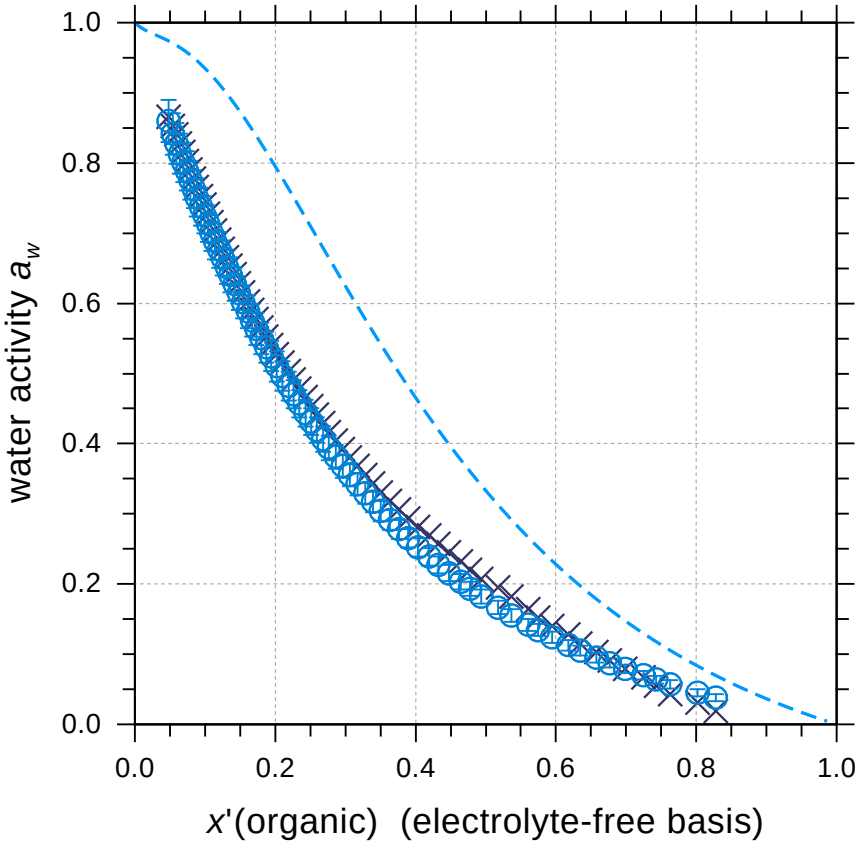


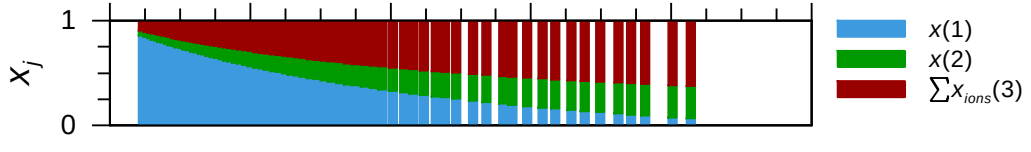
initial weighting of dataset:
$w^{init}(1047)$ = 2.000
dataset contribution to F_{obj}:
fval(1047) = 6.0688E-02
rel. contribution = 0.0289 %

Fig. S0182 (AIOMFAC_output_1057)

H_2O (1) + Levoglucosan (2) + NH_4HSO_4 (3)

Temperature: 291 K



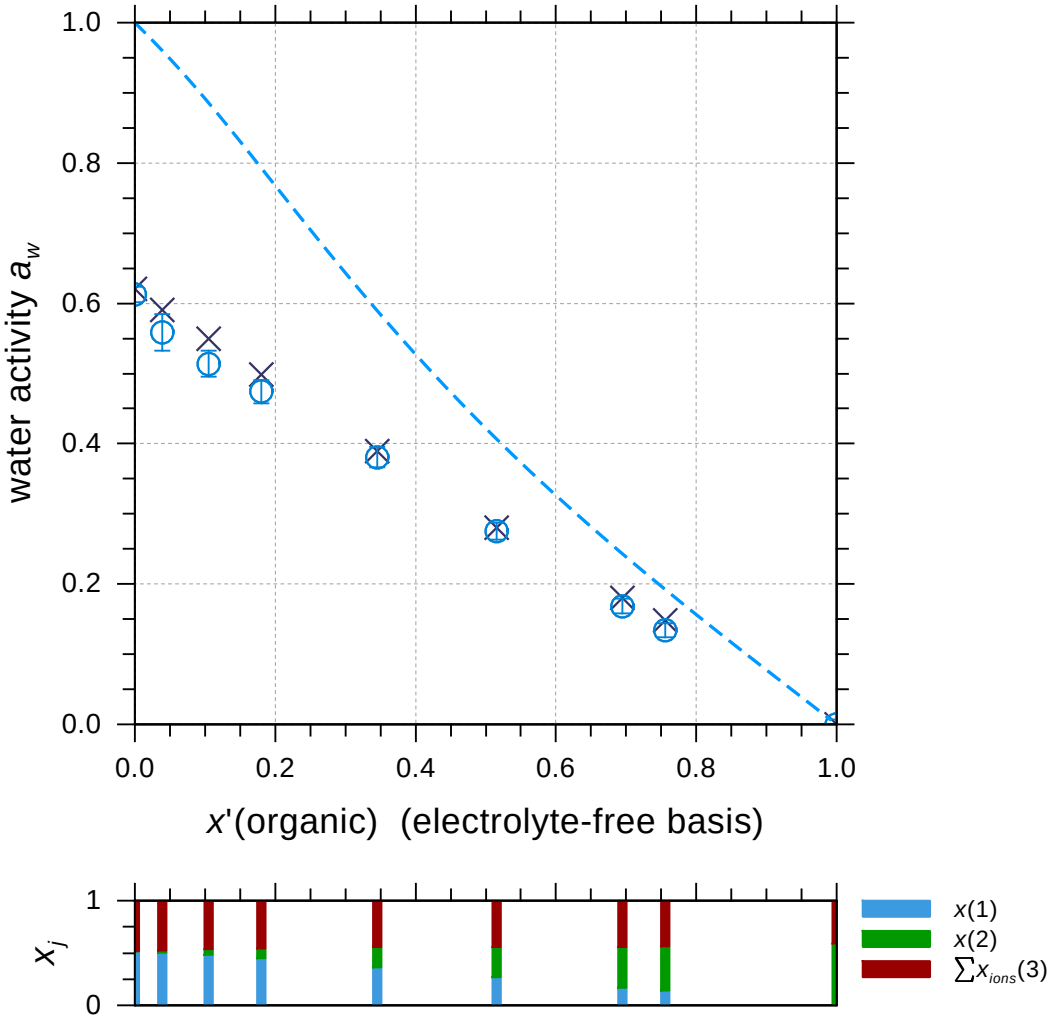


initial weighting of dataset:
$w^{init}(1057)$ = 1.000
dataset contribution to F_{obj}:
fval(1057) = 1.7181E-01
rel. contribution = 0.0817 %

Fig. S0183 (AIOMFAC_output_0072)

H_2O (1) + Glycerol (2) + NH_4NO_3 (3)

Temperature: 298 K

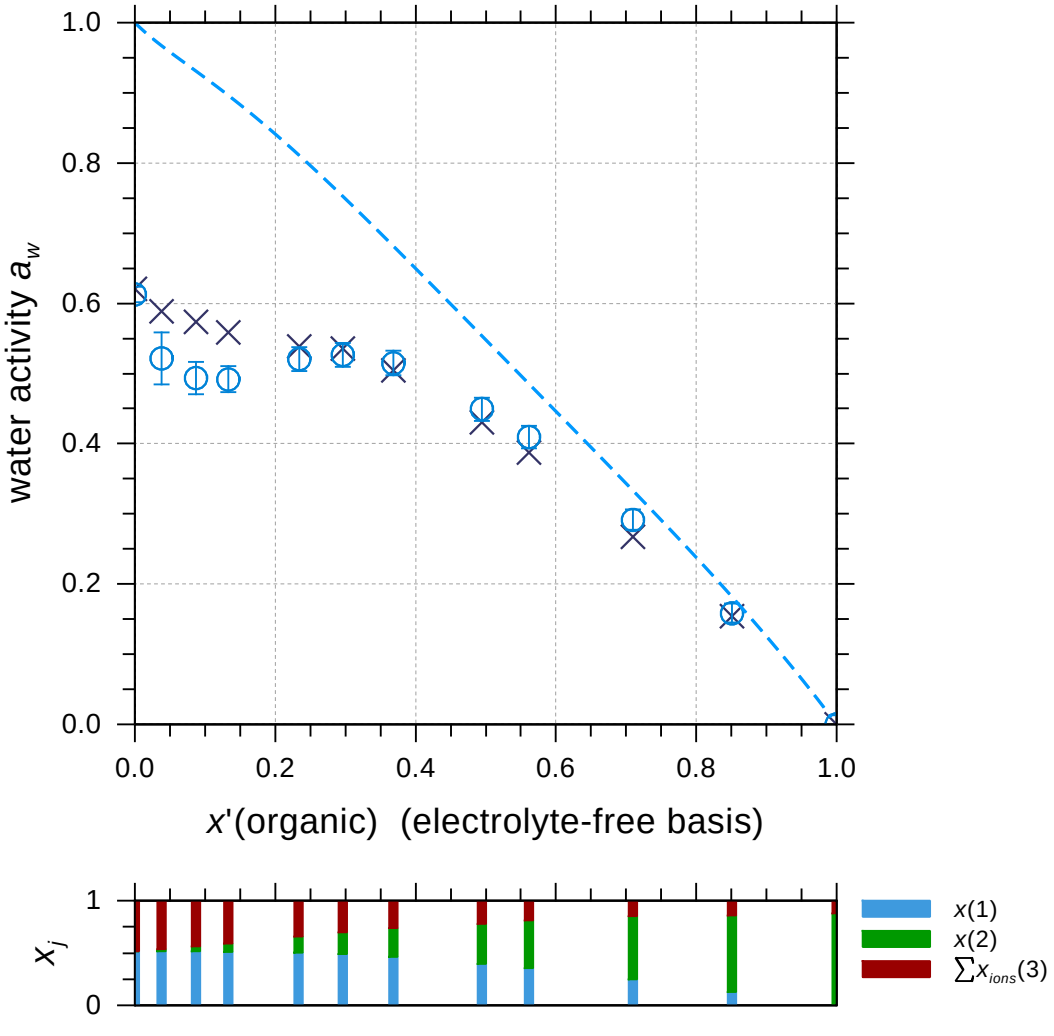


initial weighting of dataset:
w^{init}(0072) = 2.000
dataset contribution to F_{obj}:
fval(0072) = 4.2274E-02
rel. contribution = 0.0201 %

Fig. S0184 (AIOMFAC_output_0073)

H_2O (1) + 1,4-Butanediol (2) + NH_4NO_3 (3)

Temperature: 298 K

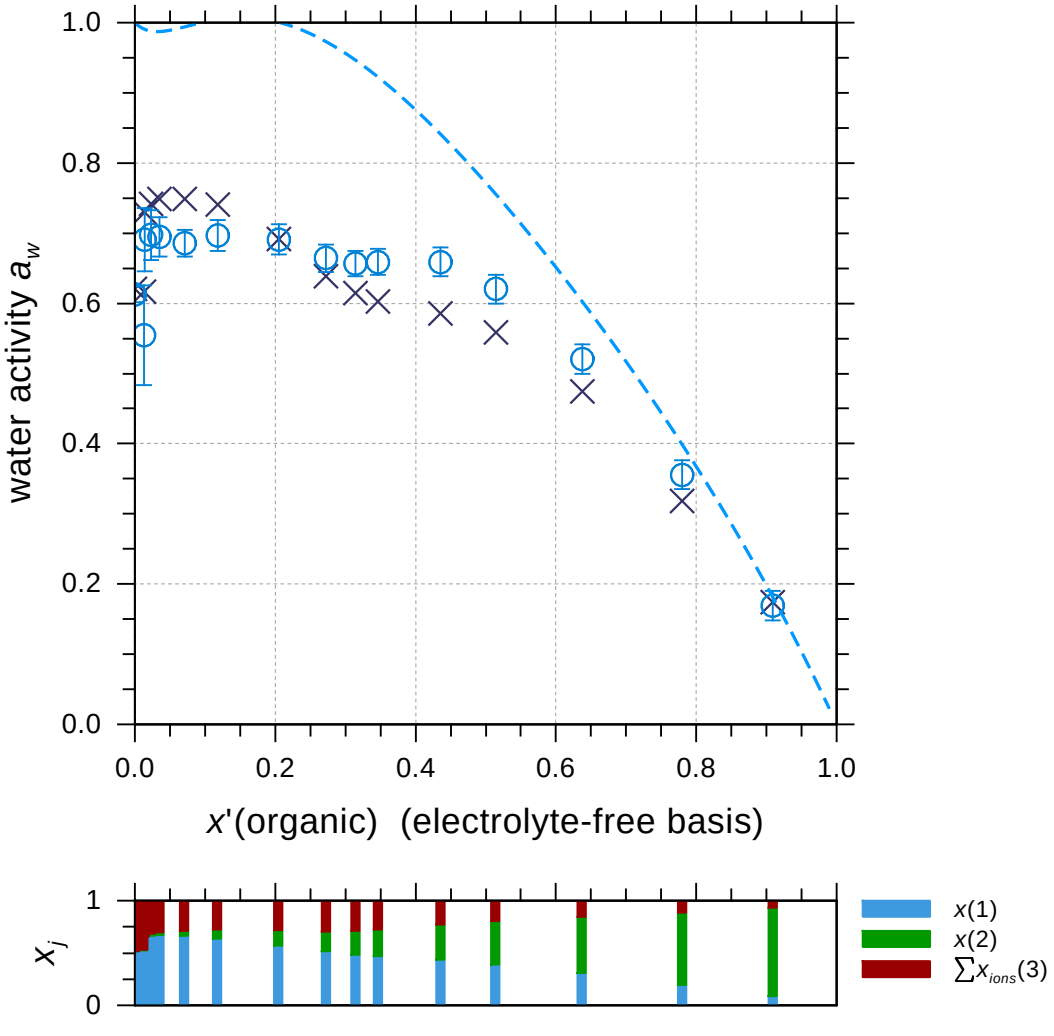


initial weighting of dataset:
$w^{init}(0073)$ = 2.000
dataset contribution to F_{obj}:
fval(0073) = 9.7647E-02
rel. contribution = 0.0464 %

Fig. S0185 (AIOMFAC_output_0074)

H_2O (1) + 1,2-Hexanediol (2) + NH_4NO_3 (3)

Temperature: 298 K

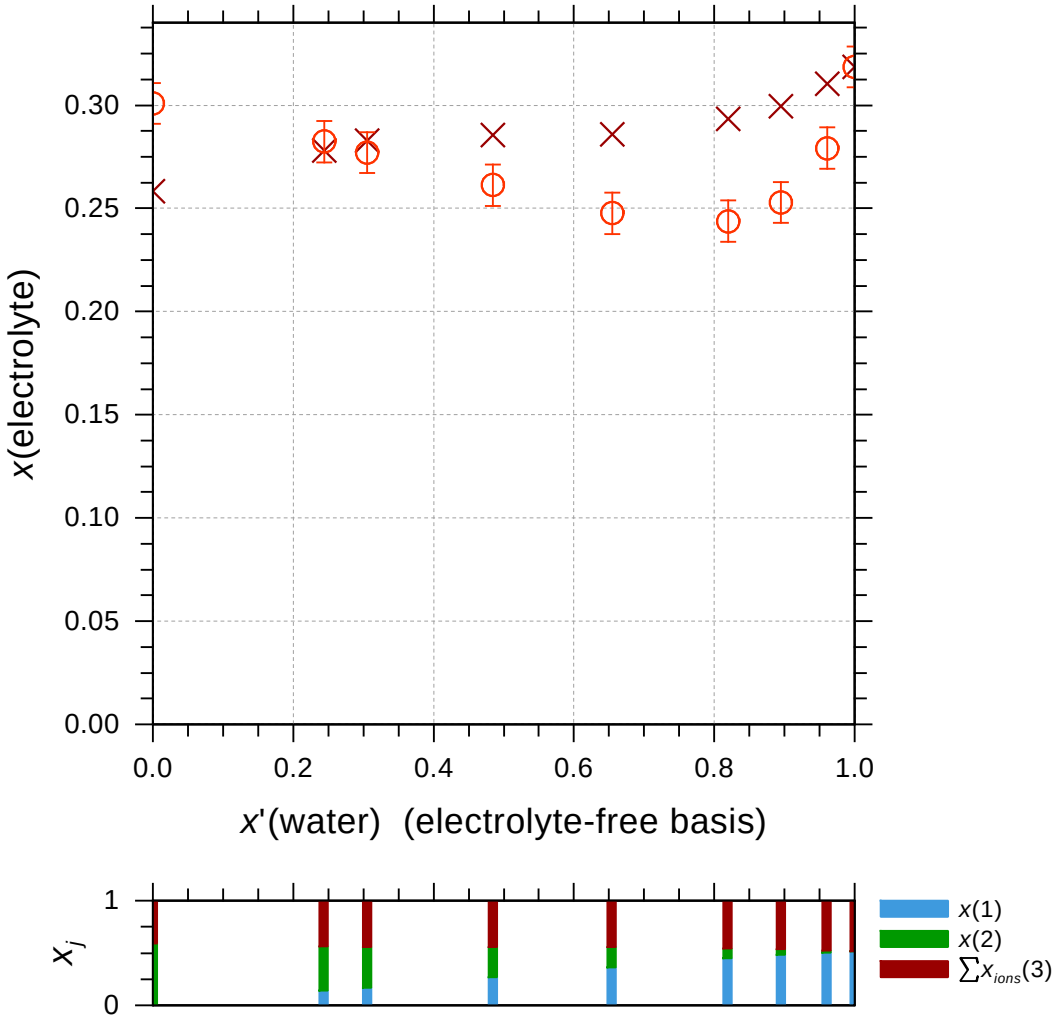


initial weighting of dataset:
$w^{init}(0074)$ = 2.000
dataset contribution to F_{obj}:
fval(0074) = 1.1356E-01
rel. contribution = 0.0540 %

Fig. S0186 (AIOMFAC_output_0955)

H_2O (1) + Glycerol (2) + NH_4NO_3 (3)

Temperature: 298 K

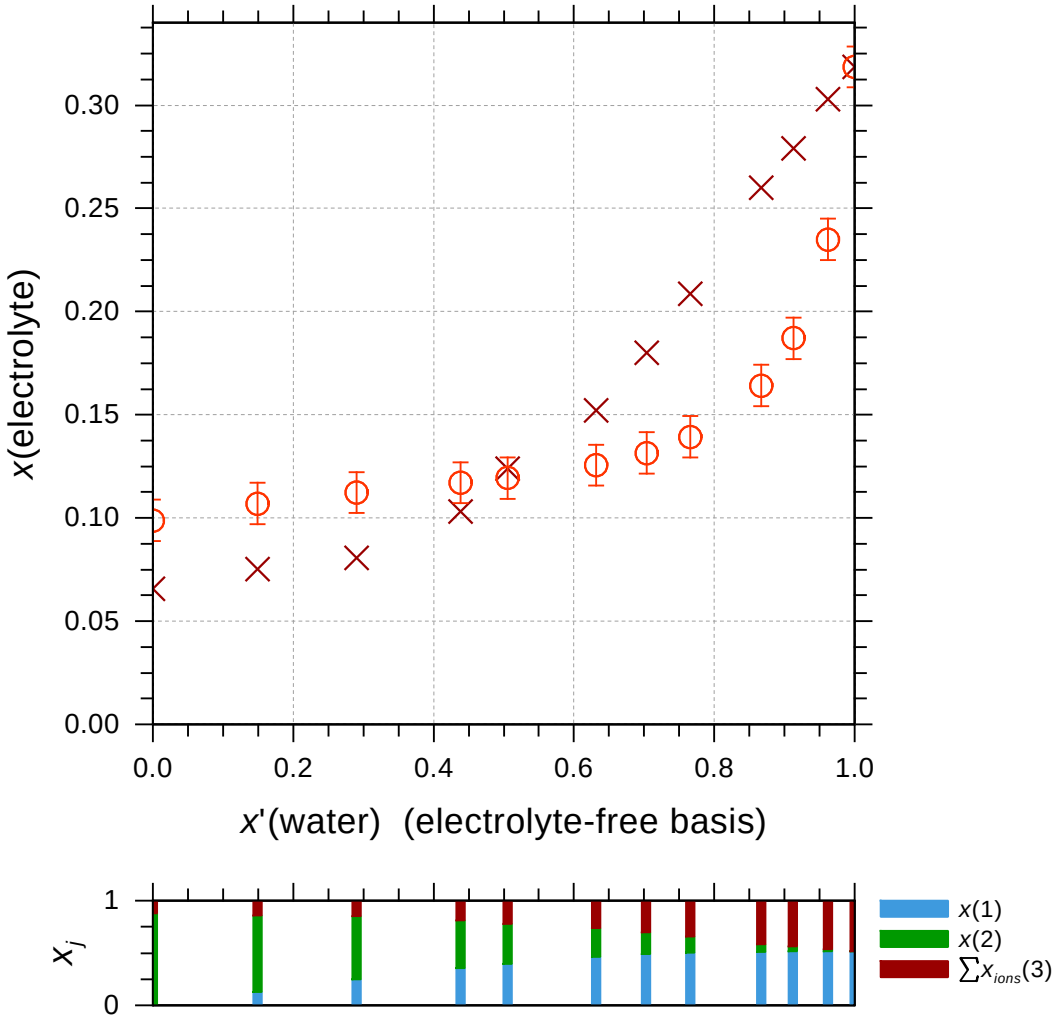


initial weighting of dataset:
$w^{init}(0955)$ = 1.000
dataset contribution to F_{obj}:
fval(0955) = 1.3917E-01
rel. contribution = 0.0662 %

Fig. S0187 (AIOMFAC_output_0956)

H_2O (1) + 1,4-Butanediol (2) + NH_4NO_3 (3)

Temperature: 298 K

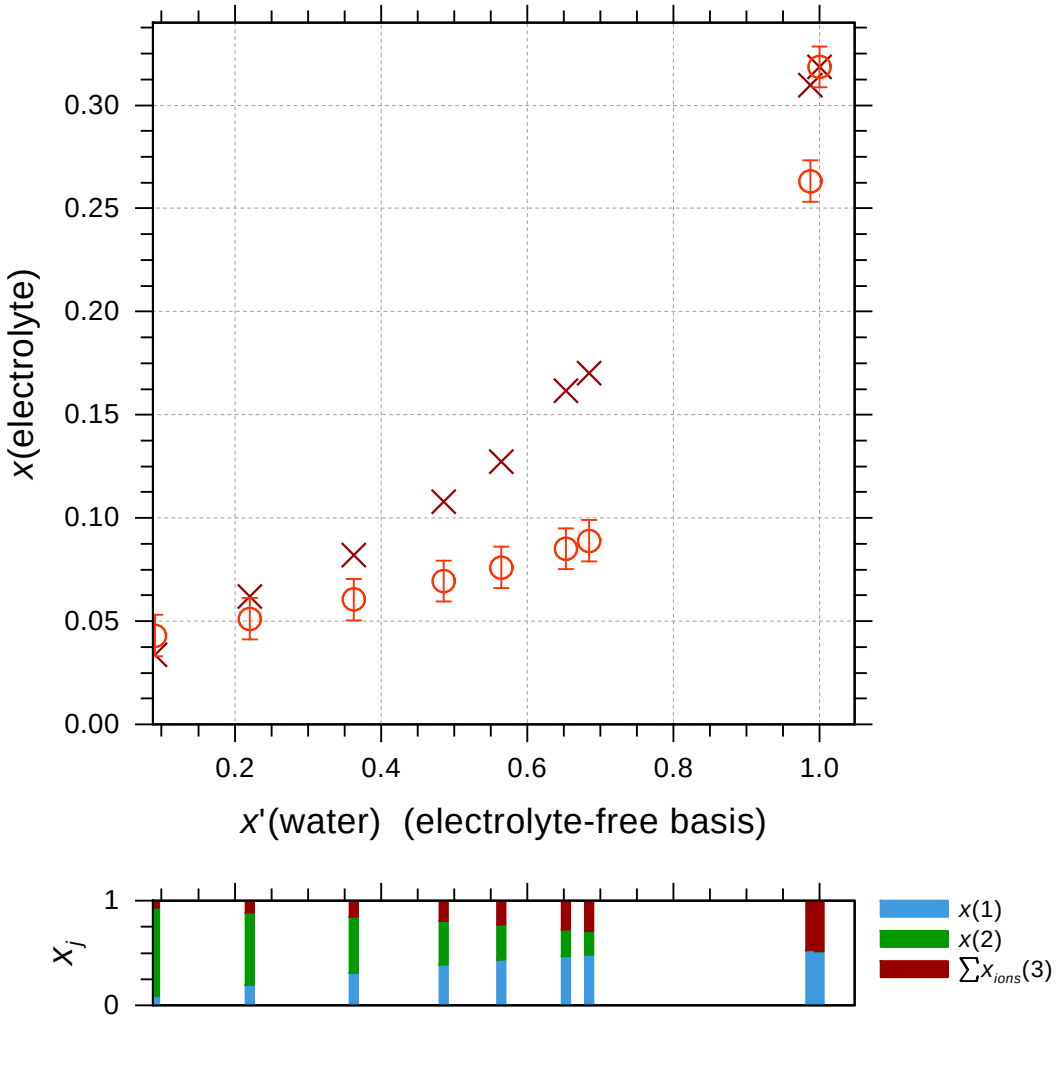


initial weighting of dataset:
$w^{init}(0956)$ = 1.000
dataset contribution to F_{obj}:
fval(0956) = 8.6384E-01
rel. contribution = 0.4108 %

Fig. S0188 (AIOMFAC_output_0957)

H_2O (1) + 1,2-Hexanediol (2) + NH_4NO_3 (3)

Temperature: 298 K

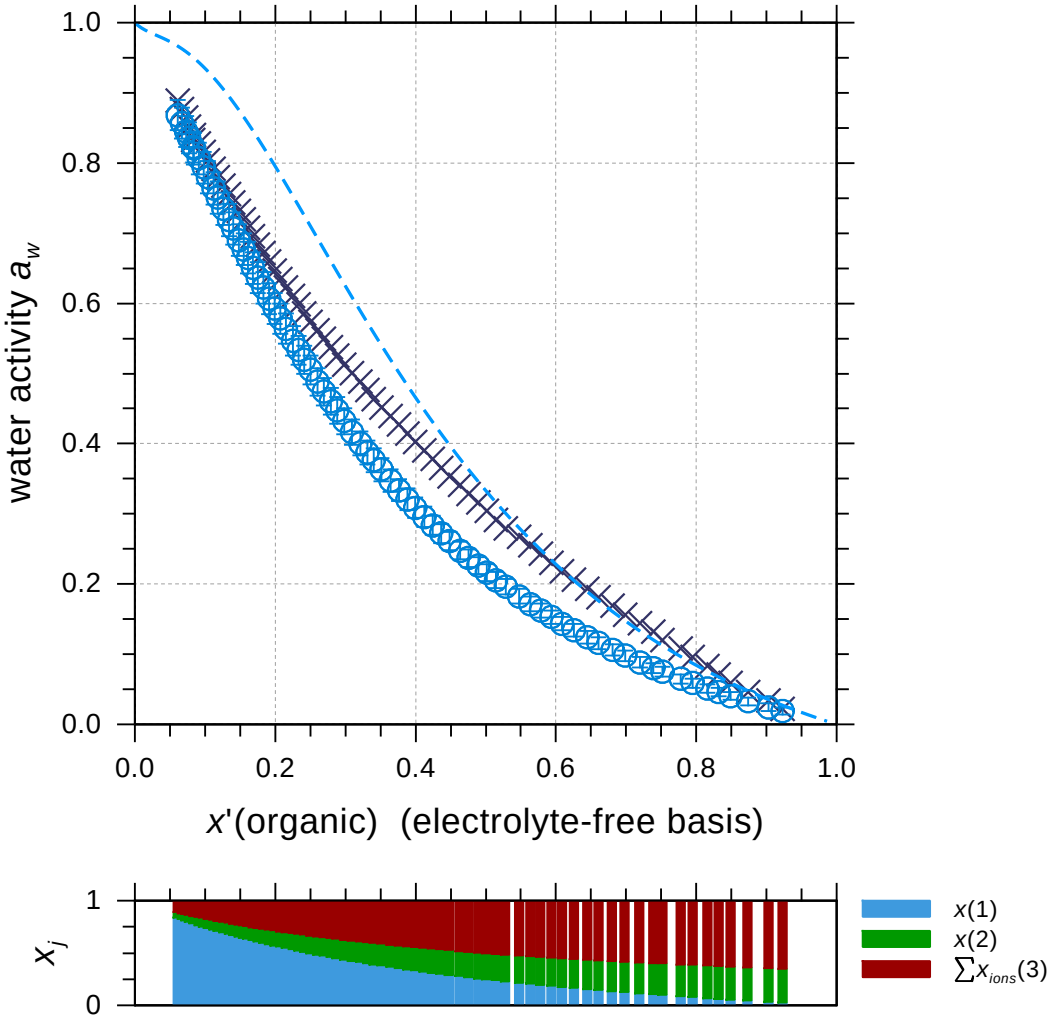


initial weighting of dataset:
$w^{init}(0957)$ = 1.000
dataset contribution to F_{obj}:
fval(0957) = 8.4495E-01
rel. contribution = 0.4018 %

Fig. S0189 (AIOMFAC_output_1056)

H_2O (1) + Levoglucosan (2) + NH_4NO_3 (3)

Temperature: 291 K

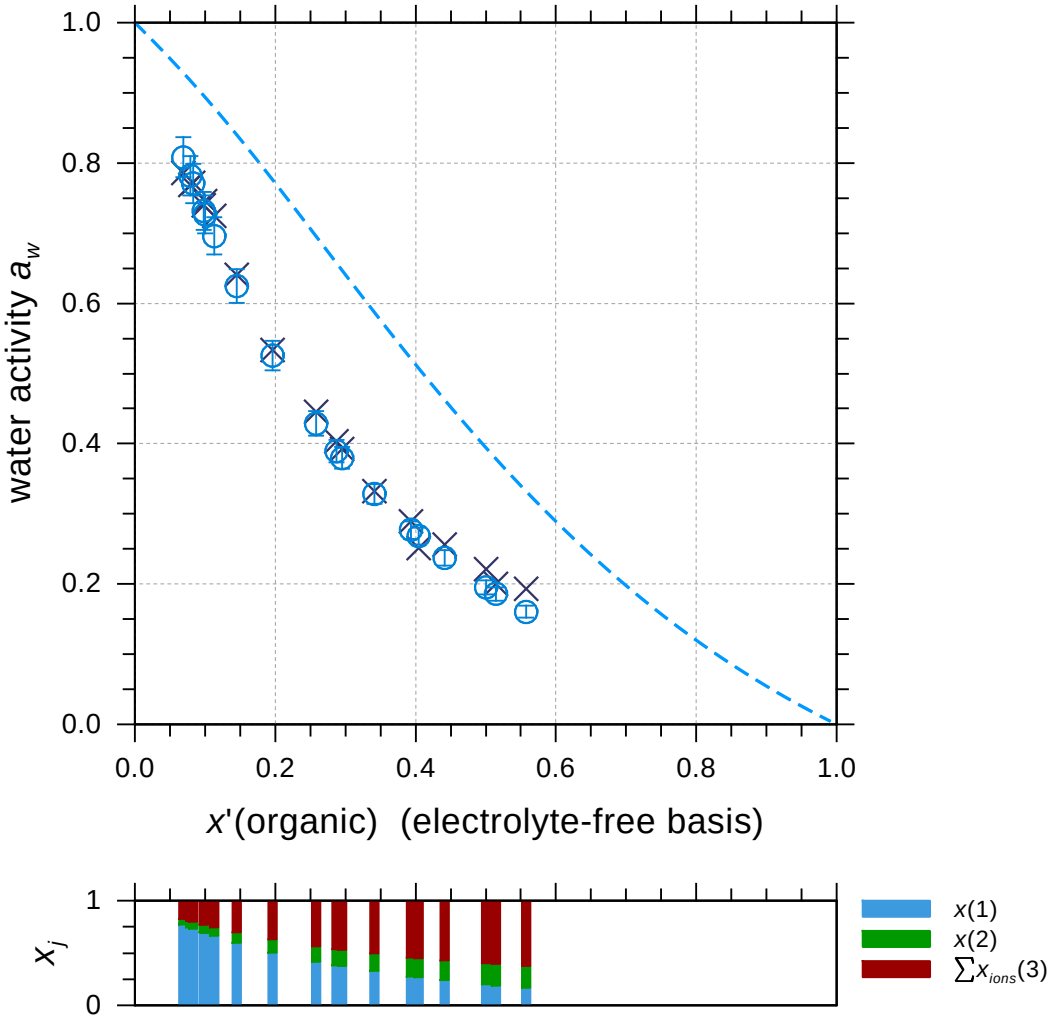


initial weighting of dataset:
w^{init}(1056) = 1.000
dataset contribution to F_{obj}:
fval(1056) = 4.7793E-01
rel. contribution = 0.2273 %

Fig. S0190 (AIOMFAC_output_0254)

H_2O (1) + Malonic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

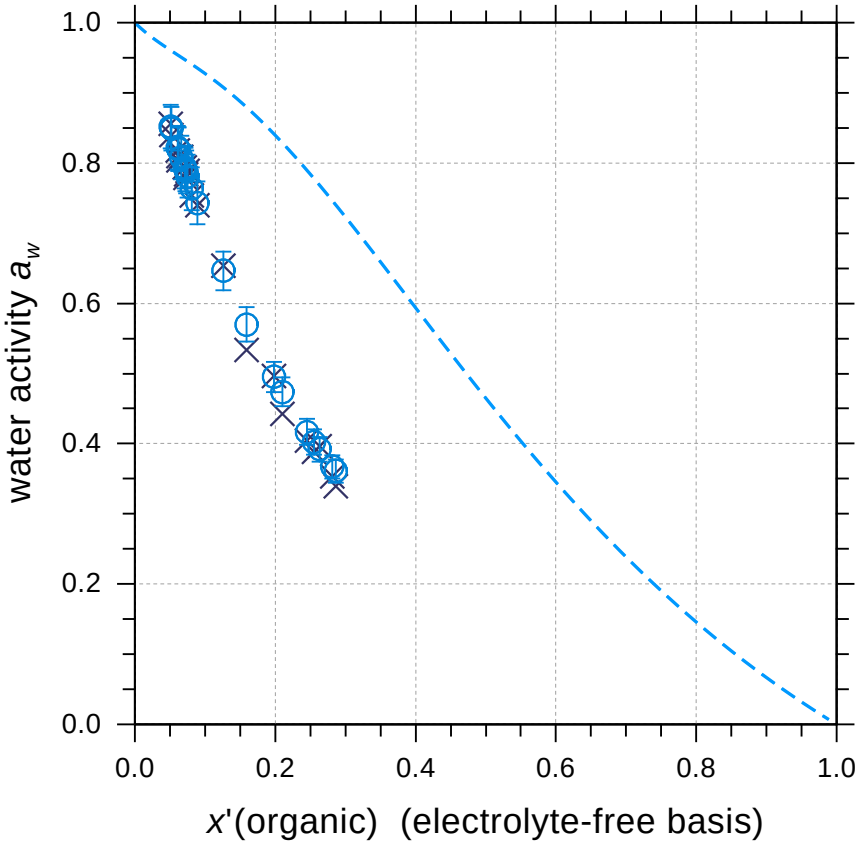


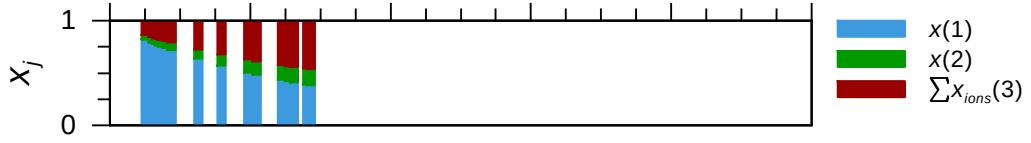
initial weighting of dataset:
$w^{init}(0254)$ = 1.000
dataset contribution to F_{obj}:
fval(0254) = 3.3853E-02
rel. contribution = 0.0161 %

Fig. S0191 (AIOMFAC_output_0255)

H_2O (1) + Glutaric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K





left y-axis:

× (NH4)2SO4+GlutaricAcid+Water_EDB-aw_Ling

○ AIOMFAC water activity a_w

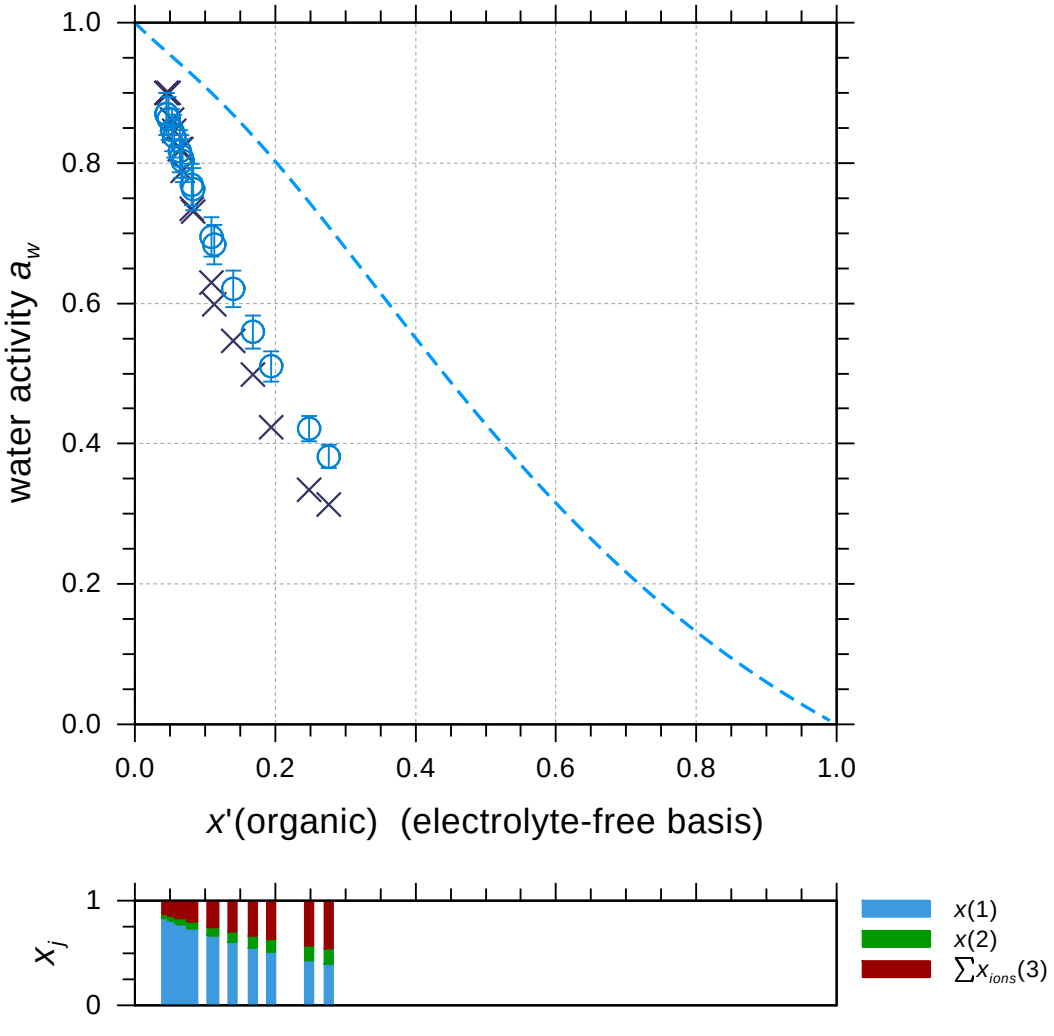
– – AIOMFAC electrolyte-free solution a_w

initial weighting of dataset:
$w^{init}(0255)$ = 1.000
dataset contribution to F_{obj}:
fval(0255) = 8.3894E-03
rel. contribution = 0.0040 %

Fig. S0192 (AIOMFAC_output_0256)

H_2O (1) + Succinic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

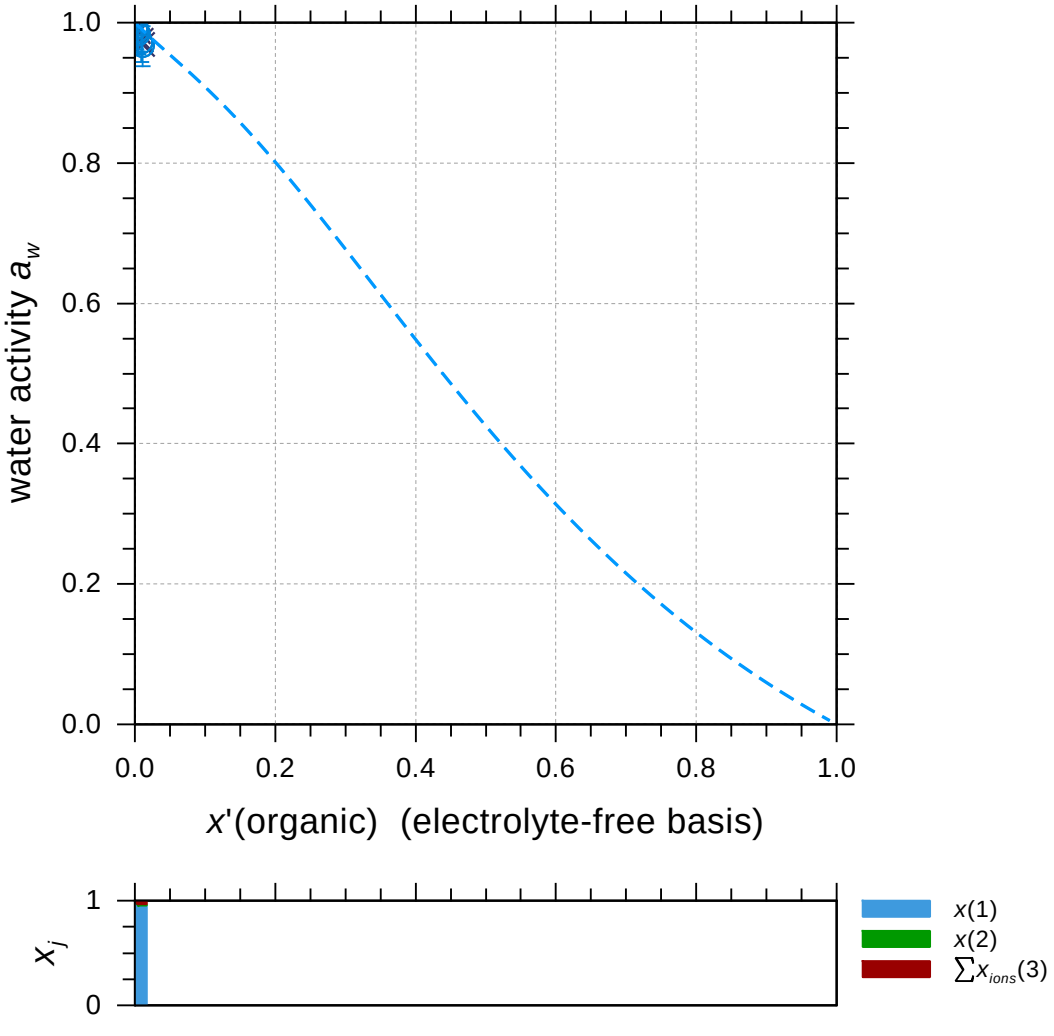


initial weighting of dataset:
w^{init}(0256) = 1.000
dataset contribution to F_{obj}:
fval(0256) = 1.2339E-01
rel. contribution = 0.0587 %

Fig. S0193 (AIOMFAC_output_0257)

H_2O (1) + Succinic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 295 K

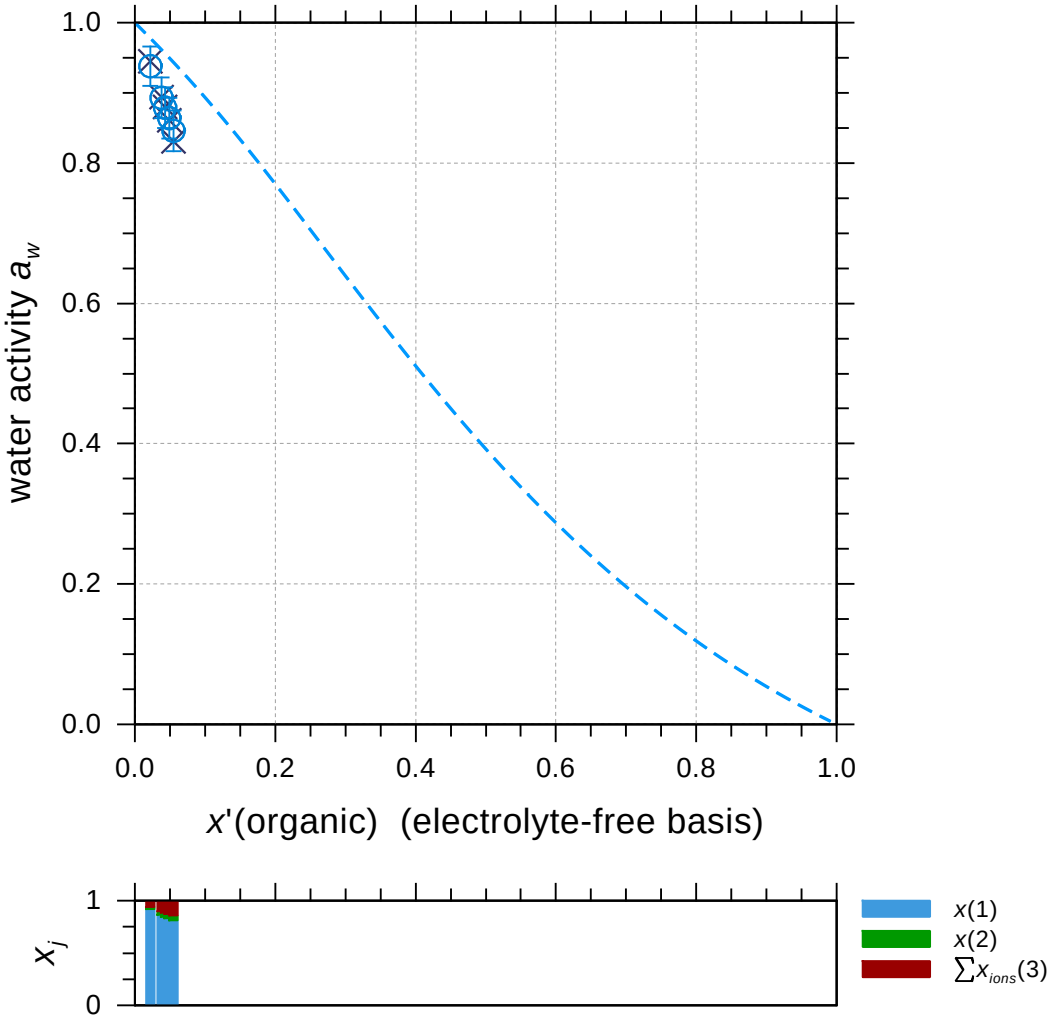


initial weighting of dataset:
w^{init}(0257) = 2.000
dataset contribution to F_{obj}:
fval(0257) = 5.7813E-05
rel. contribution = 0.0000 %

Fig. S0194 (AIOMFAC_output_0258)

H_2O (1) + Malonic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 295 K

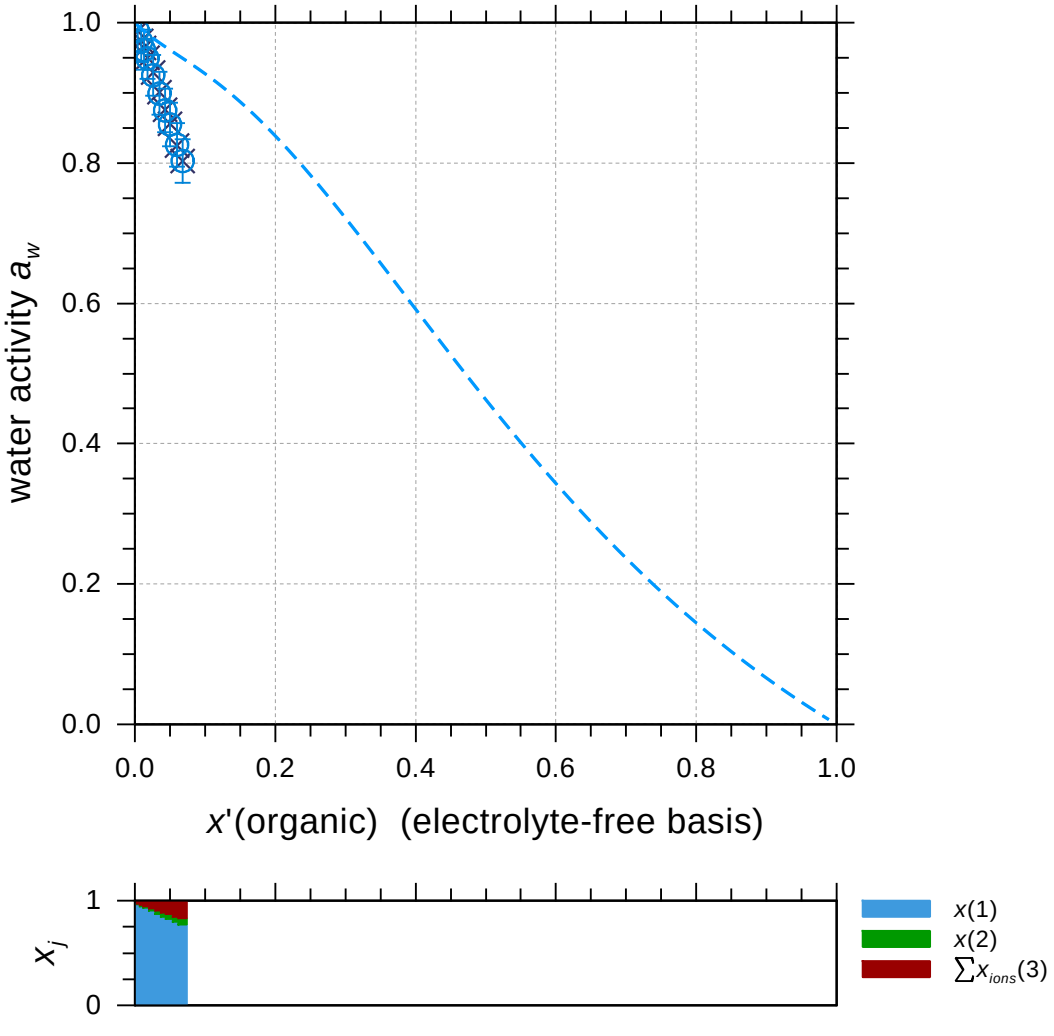


initial weighting of dataset:
$w^{init}(0258)$ = 2.000
dataset contribution to F_{obj}:
fval(0258) = 7.3458E-04
rel. contribution = 0.0003 %

Fig. S0195 (AIOMFAC_output_0259)

H_2O (1) + Glutaric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 295 K

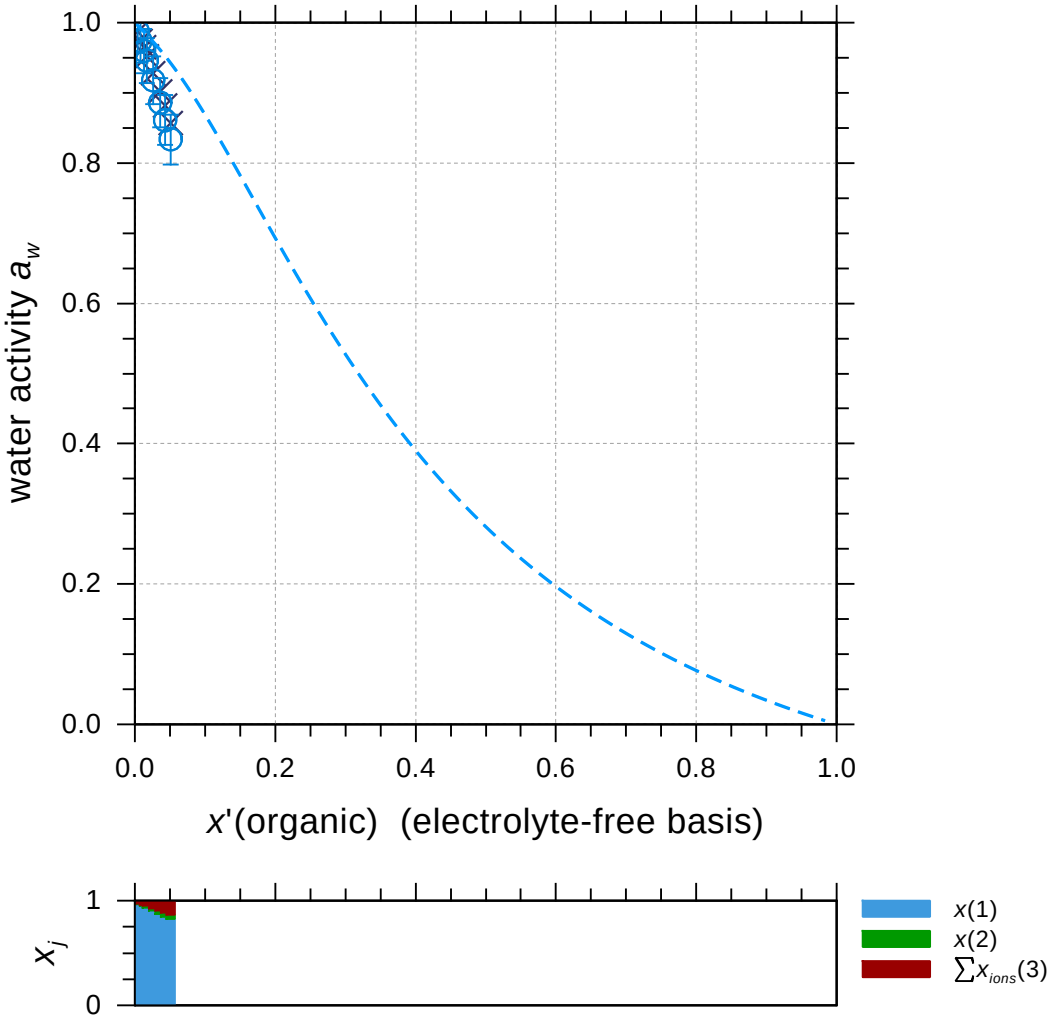


initial weighting of dataset:
$w^{init}(0259)$ = 2.000
dataset contribution to F_{obj}:
fval(0259) = 7.4522E-05
rel. contribution = 0.0000 %

Fig. S0196 (AIOMFAC_output_0260)

H_2O (1) + Citric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 295 K

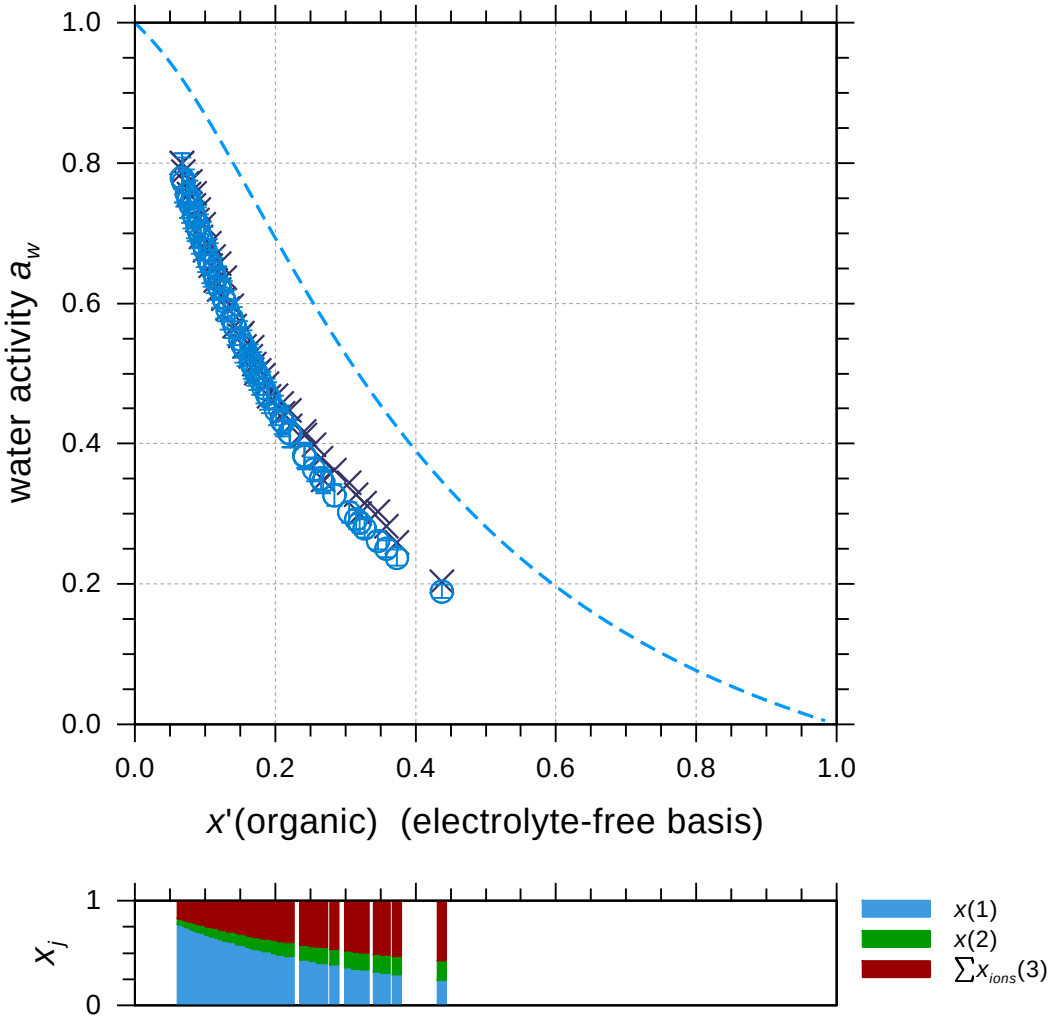


initial weighting of dataset:
$w^{init}(0260)$ = 2.000
dataset contribution to F_{obj}:
fval(0260) = 3.3482E-03
rel. contribution = 0.0016 %

Fig. S0197 (AIOMFAC_output_0261)

H_2O (1) + Citric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 295 K

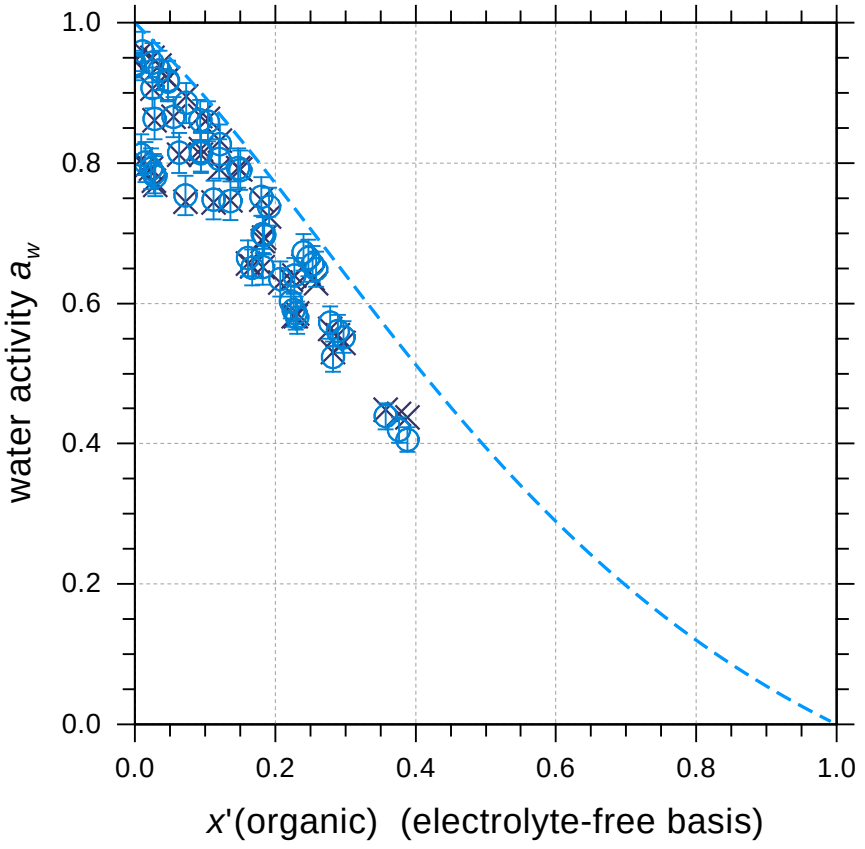


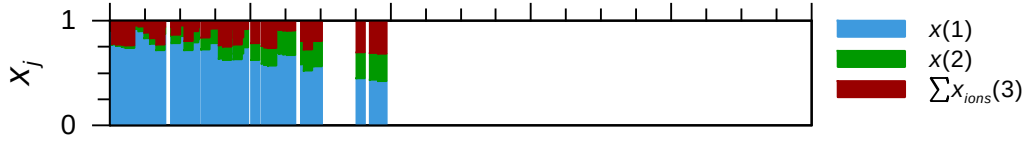
initial weighting of dataset:
$w^{init}(0261)$ = 0.100
dataset contribution to F_{obj}:
fval(0261) = 2.6471E-03
rel. contribution = 0.0013 %

Fig. S0198 (AIOMFAC_output_0269)

H_2O (1) + Malonic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K





left y-axis:

(NH4)2SO4+MalonicAcid+Water_aw_Salcedo

AIOMFAC water activity a_w

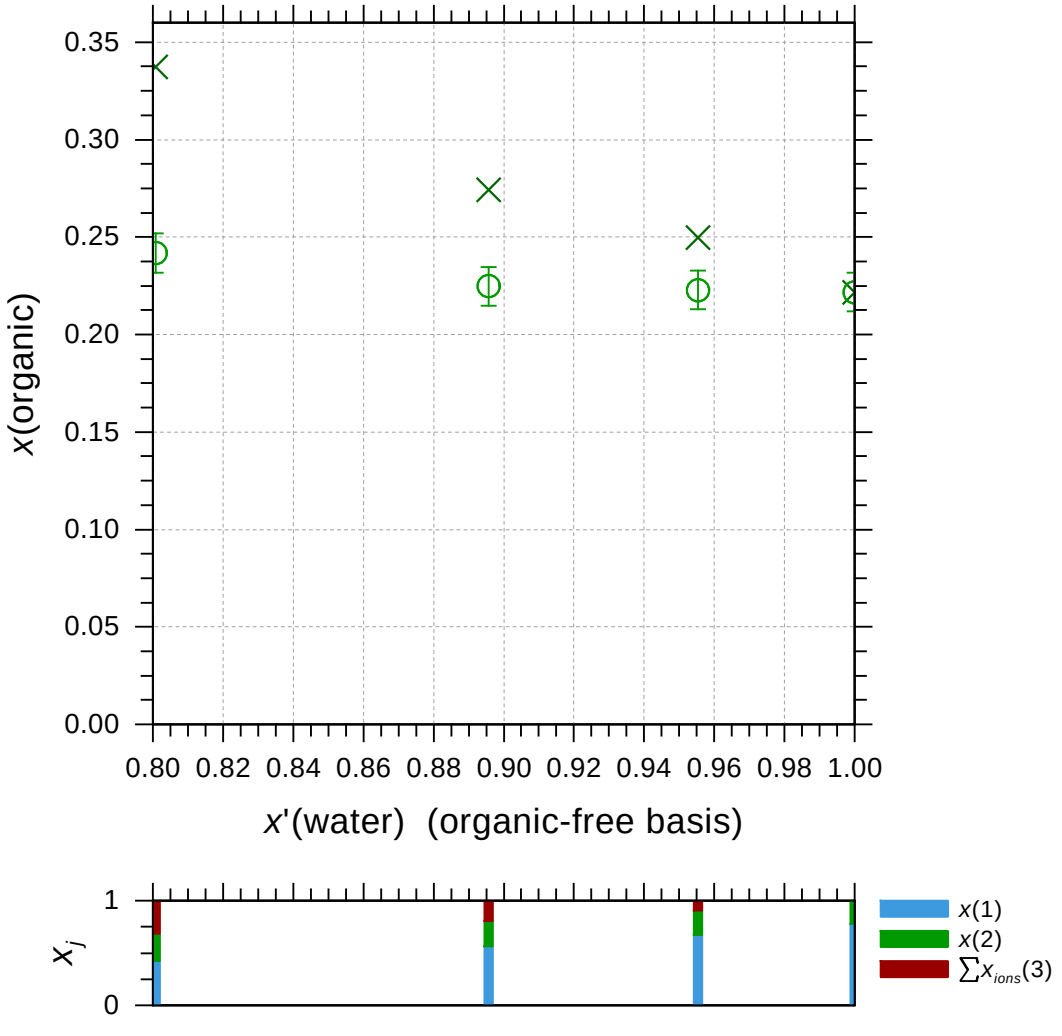
AIOMFAC electrolyte-free solution a_w

initial weighting of dataset:
$w^{init}(0269)$ = 2.000
dataset contribution to F_{obj}:
fval(0269) = 6.3668E-03
rel. contribution = 0.0030 %

Fig. S0199 (AIOMFAC_output_0270)

H_2O (1) + Malonic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

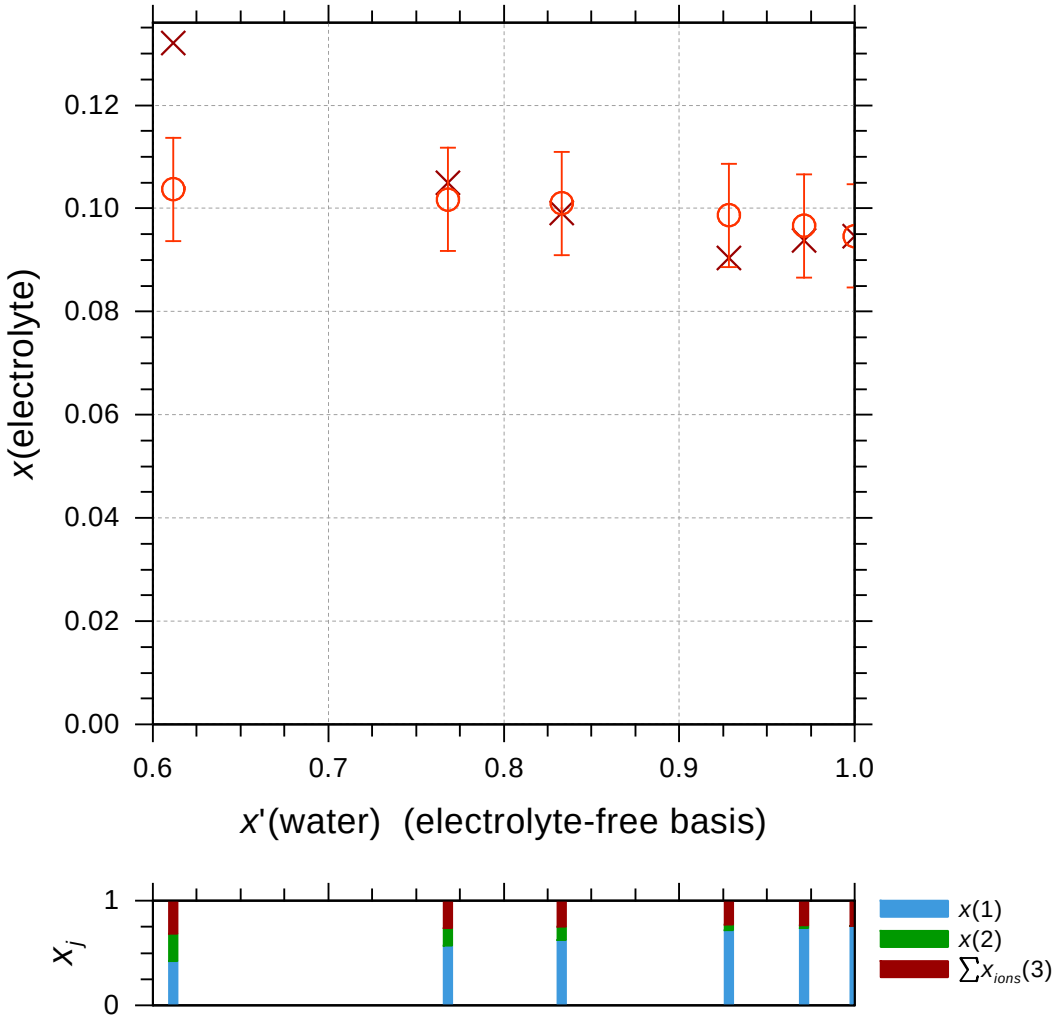


initial weighting of dataset:
$w^{init}(0270)$ = 1.000
dataset contribution to F_{obj}:
fval(0270) = 1.6476E-01
rel. contribution = 0.0783 %

Fig. S0200 (AIOMFAC_output_0271)

H_2O (1) + Malonic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

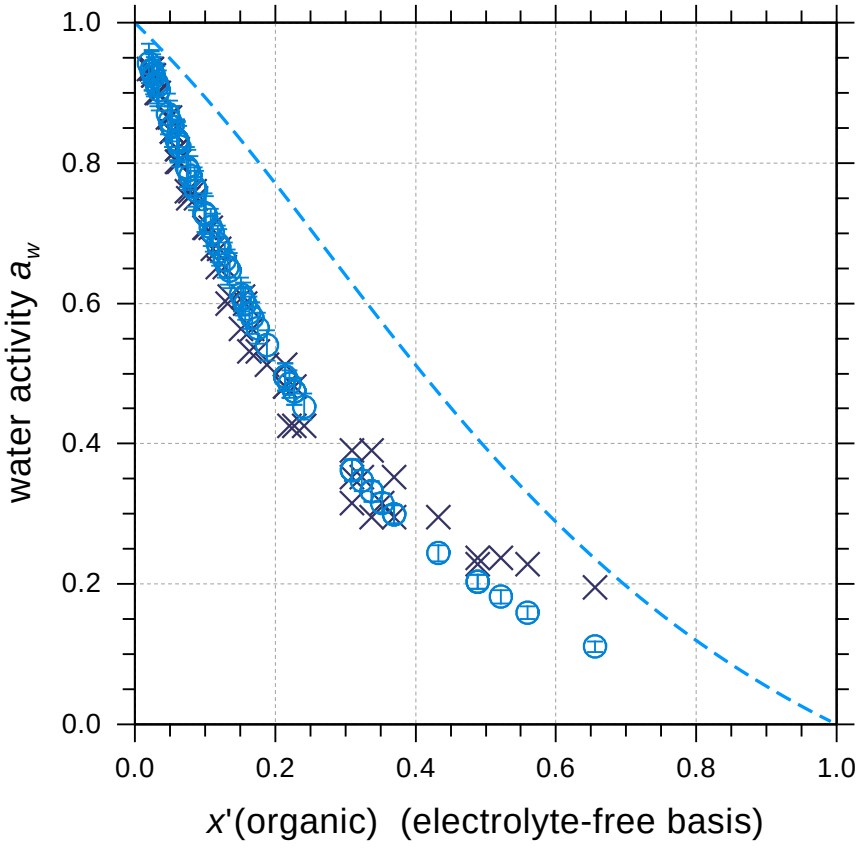


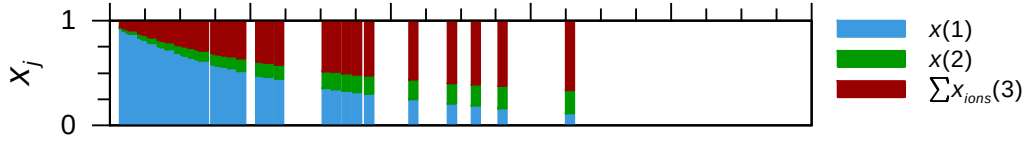
initial weighting of dataset:
$w^{init}(0271)$ = 1.000
dataset contribution to F_{obj}:
fval(0271) = 5.0439E-02
rel. contribution = 0.0240 %

Fig. S0201 (AIOMFAC_output_0275)

H_2O (1) + Malonic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 297 K



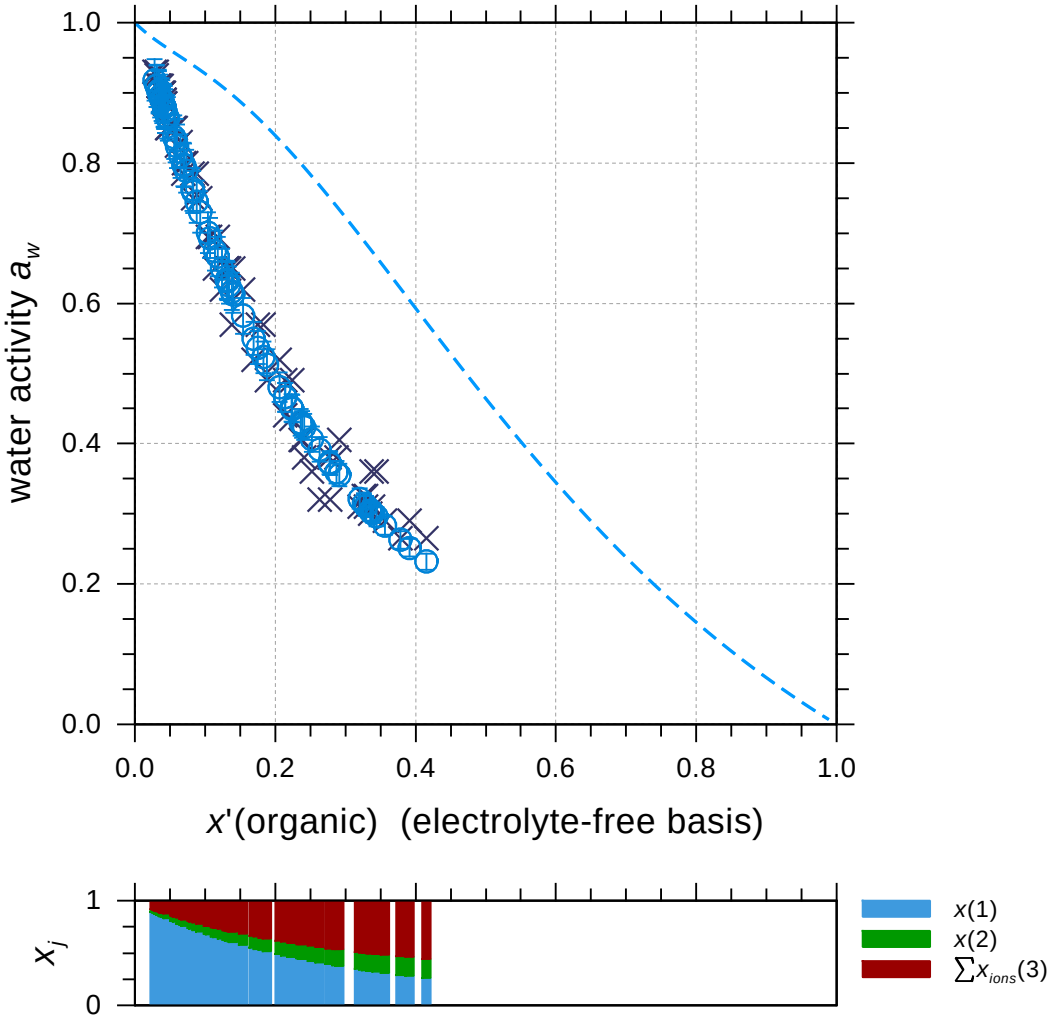


initial weighting of dataset:
$w^{init}(0275)$ = 0.200
dataset contribution to F_{obj}:
fval(0275) = 1.7458E-02
rel. contribution = 0.0083 %

Fig. S0202 (AIOMFAC_output_0276)

H_2O (1) + Glutaric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 297 K

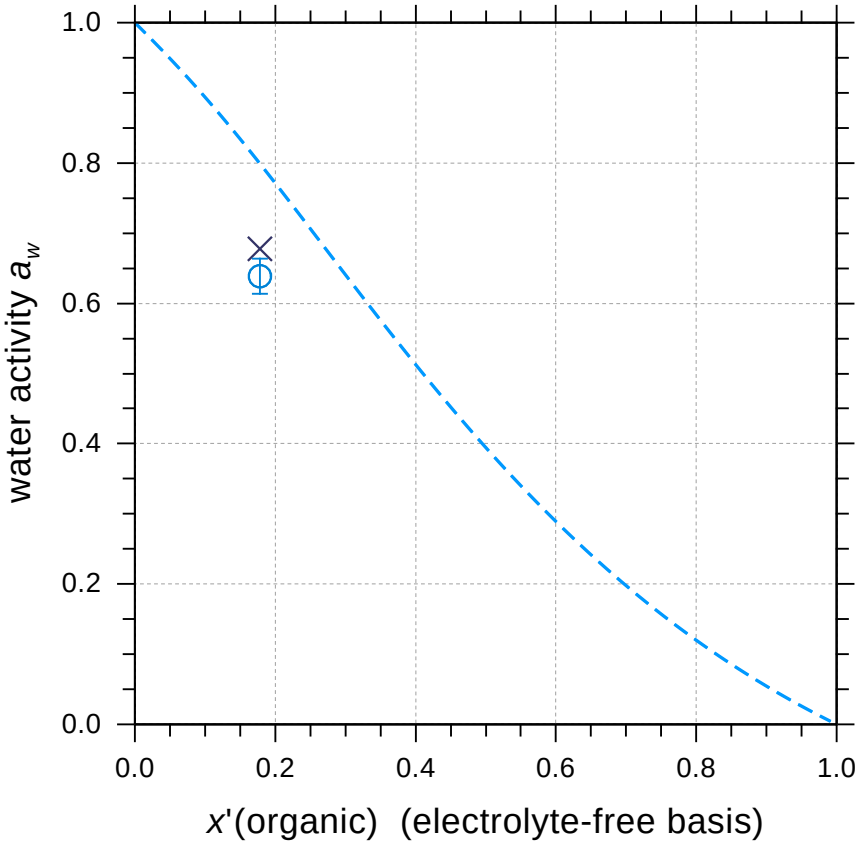


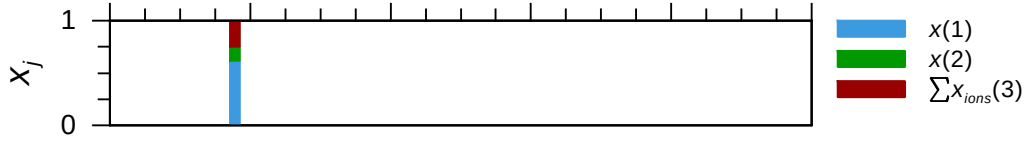
initial weighting of dataset:
$w^{init}(0276)$ = 0.200
dataset contribution to F_{obj}:
fval(0276) = 7.6424E-03
rel. contribution = 0.0036 %

Fig. S0203 (AIOMFAC_output_0278)

H_2O (1) + Malonic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K



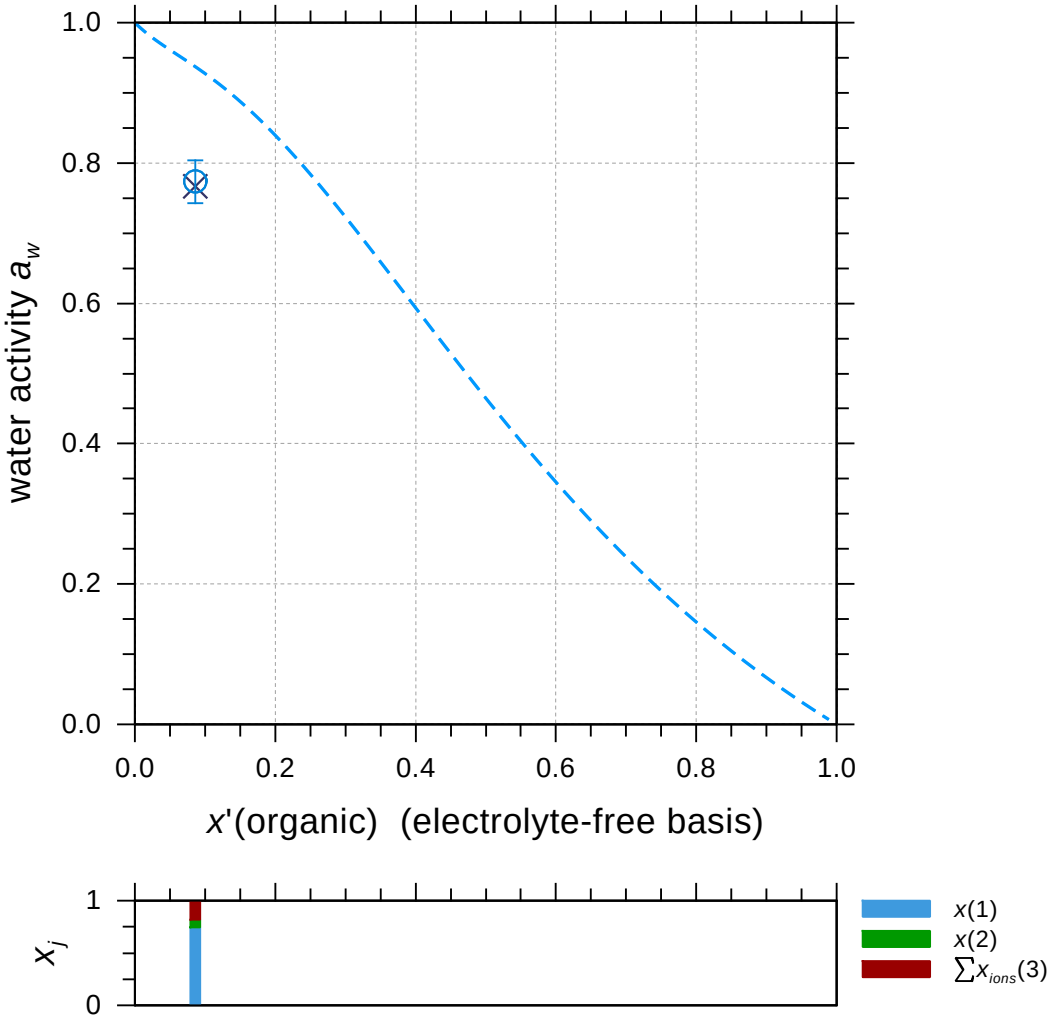


initial weighting of dataset:
$w^{init}(0278)$ = 2.000
dataset contribution to F_{obj}:
fval(0278) = 6.1292E-03
rel. contribution = 0.0029 %

Fig. S0204 (AIOMFAC_output_0279)

H_2O (1) + Glutaric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

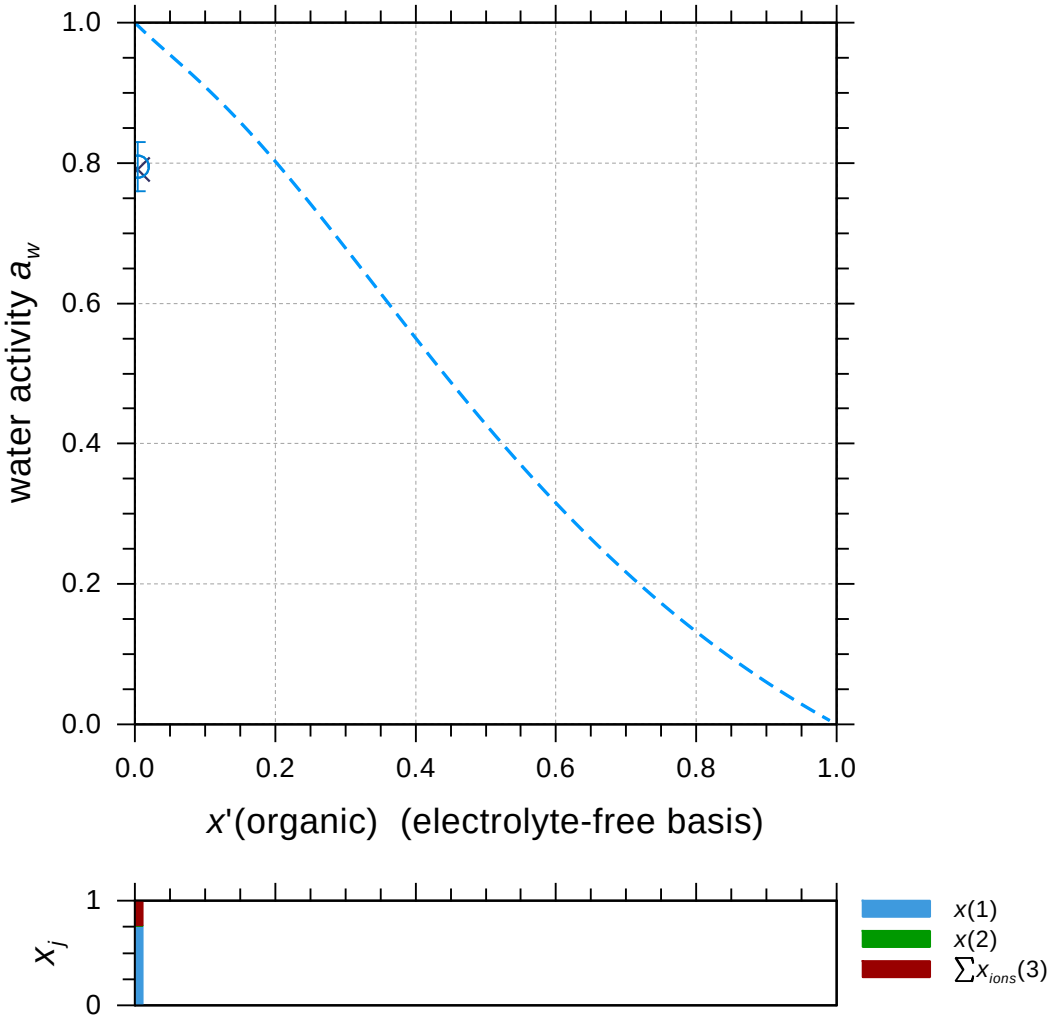


initial weighting of dataset:
$w^{init}(0279)$ = 2.000
dataset contribution to F_{obj}:
fval(0279) = 1.2439E-04
rel. contribution = 0.0001 %

Fig. S0205 (AIOMFAC_output_0280)

H_2O (1) + Succinic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

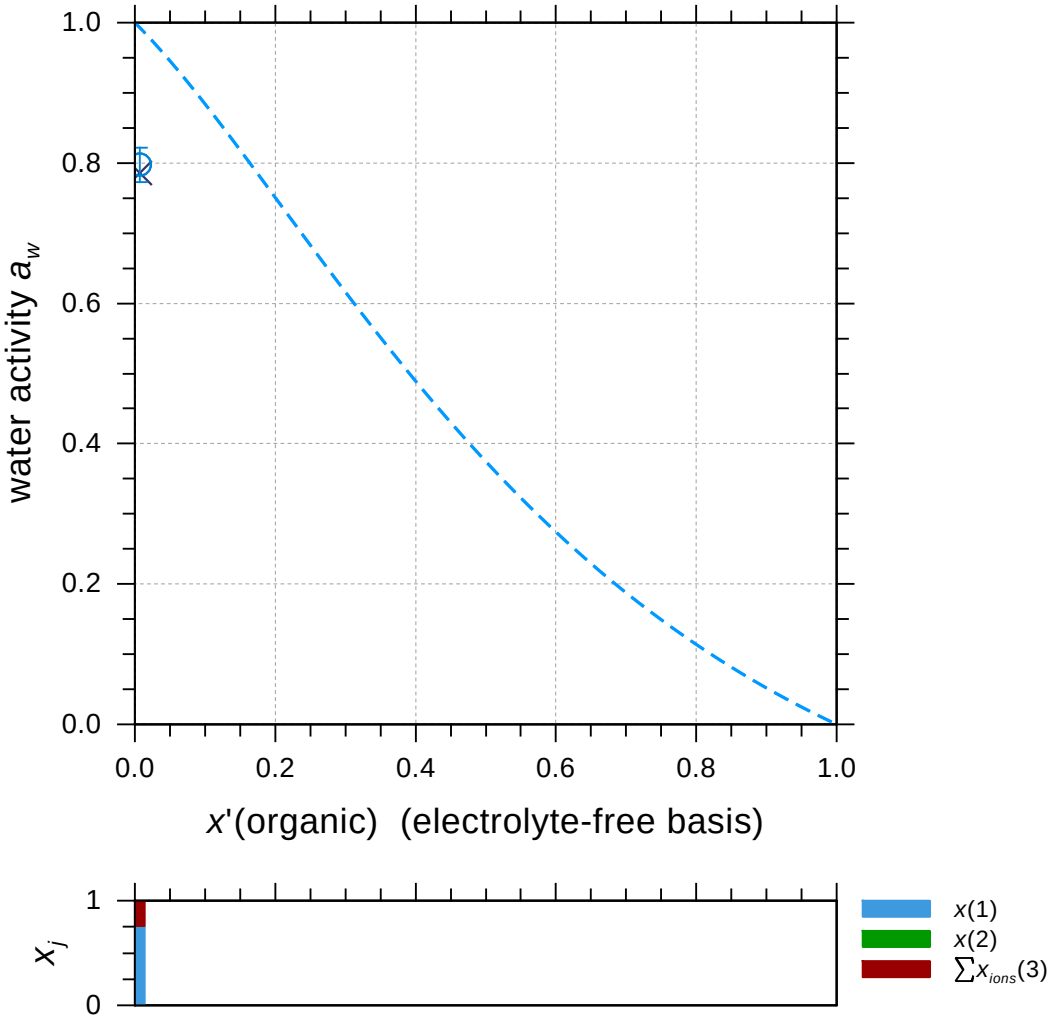


initial weighting of dataset:
w^{init}(0280) = 2.000
dataset contribution to F_{obj}:
fval(0280) = 4.3171E-05
rel. contribution = 0.0000 %

Fig. S0206 (AIOMFAC_output_0281)

H_2O (1) + Oxalic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

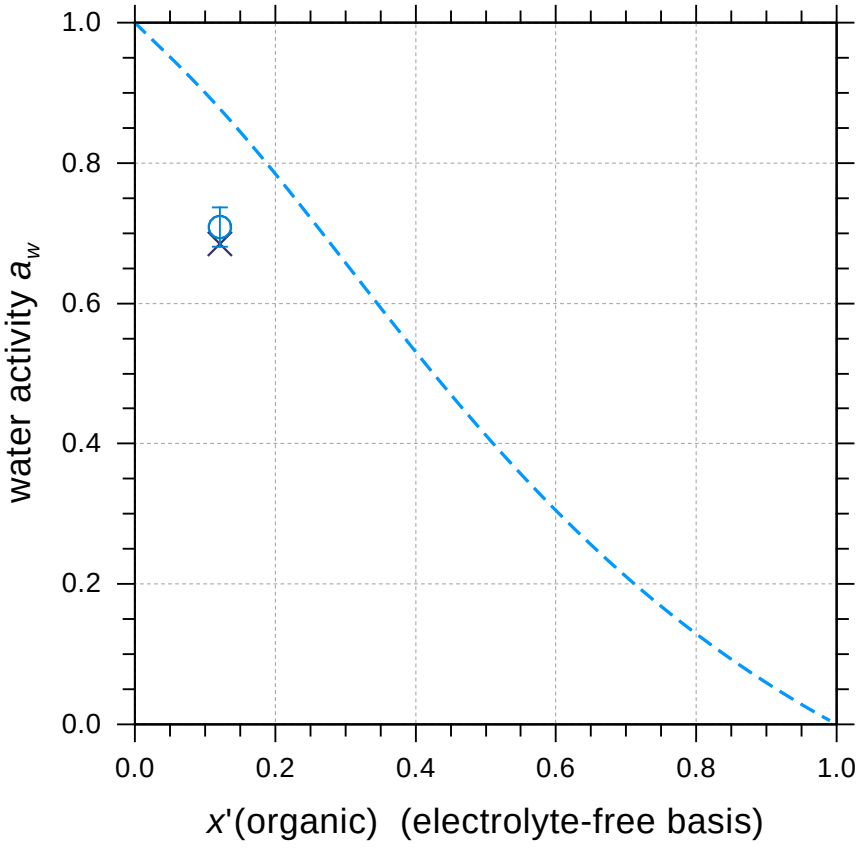


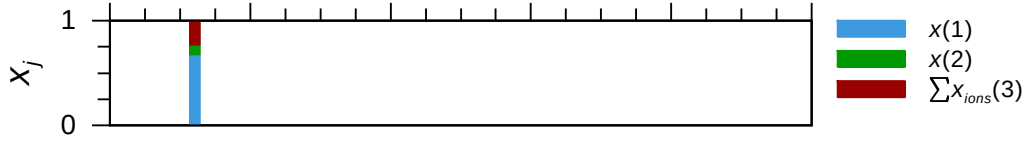
initial weighting of dataset:
$w^{init}(0281)$ = 2.000
dataset contribution to F_{obj}:
fval(0281) = 3.9555E-04
rel. contribution = 0.0002 %

Fig. S0207 (AIOMFAC_output_0282)

H_2O (1) + Maleic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K



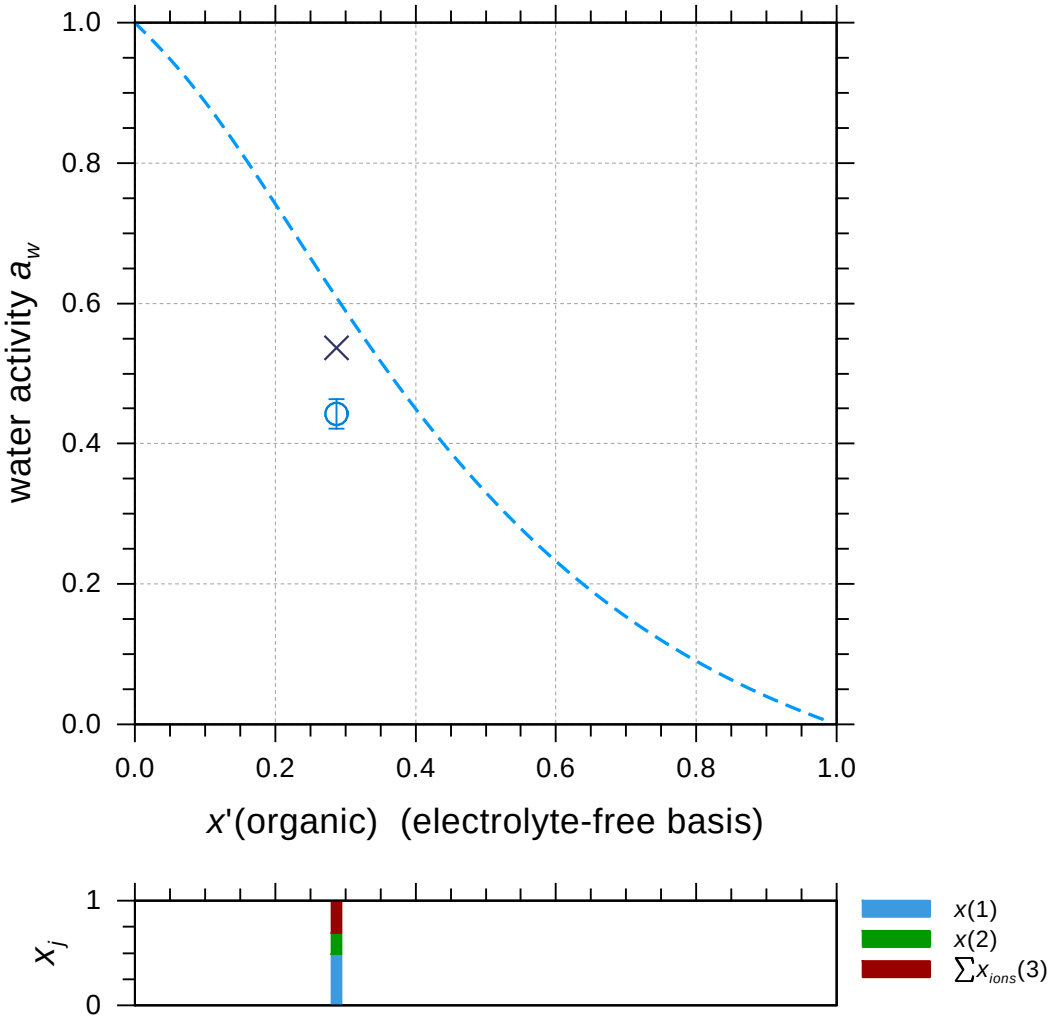


initial weighting of dataset:
$w^{init}(0282)$ = 2.000
dataset contribution to F_{obj}:
fval(0282) = 2.2059E-03
rel. contribution = 0.0010 %

Fig. S0208 (AIOMFAC_output_0283)

H_2O (1) + Malic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 298 K

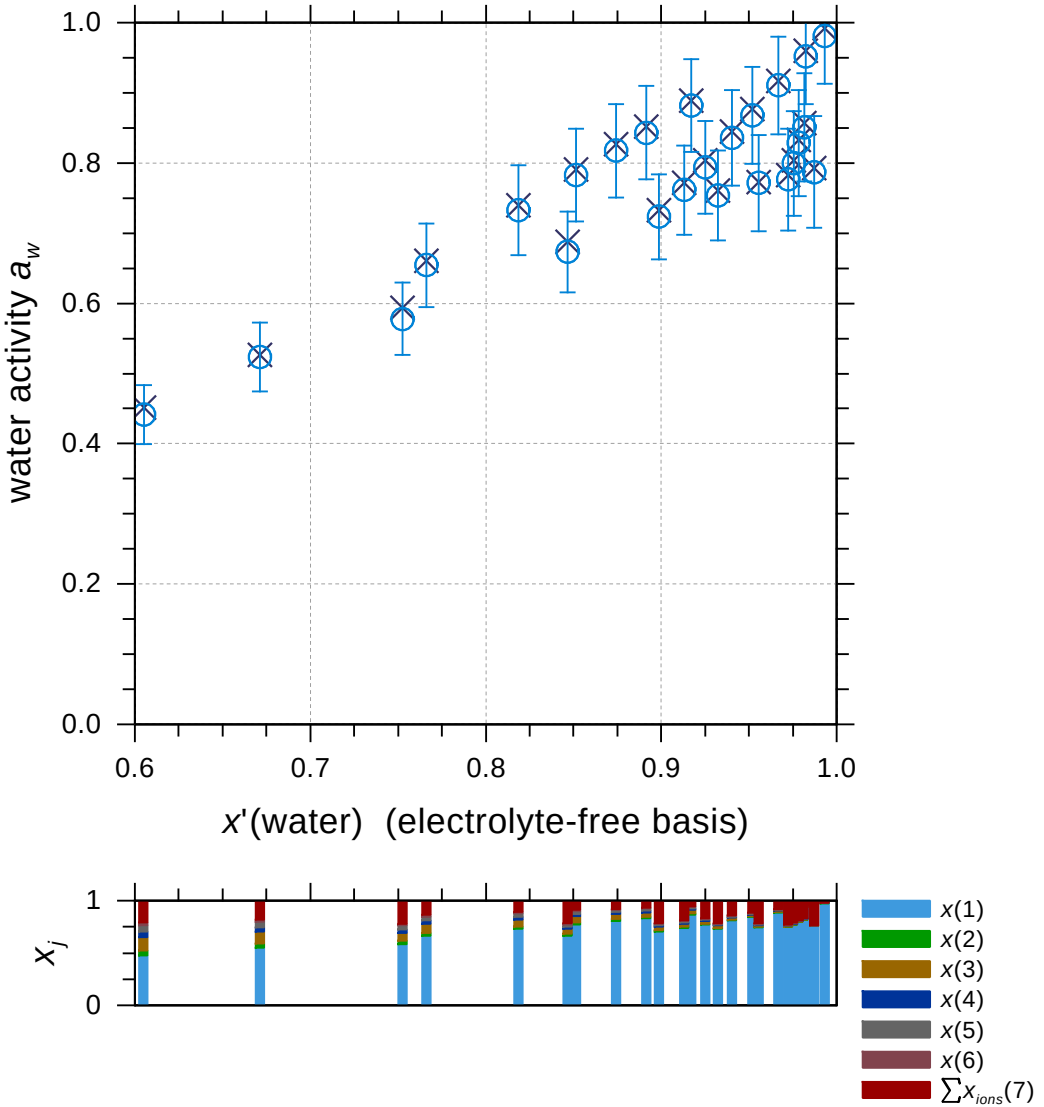


initial weighting of dataset:
w^{init}(0283) = 1.000
dataset contribution to F_{obj}:
fval(0283) = 2.8800E-02
rel. contribution = 0.0137 %

Fig. S0209 (AIOMFAC_output_0284)

H_2O (1) + Malic_acid (2) + Malonic_acid (3) + Maleic_acid (4) + Glutaric_acid (5) + Methylsuccinic_acid (6) + $(NH_4)_2SO_4$

Temperature: 298 K



initial weighting of dataset:
$w^{init}(0284)$ = 2.000
dataset contribution to F_{obj}:
fval(0284) = 2.4067E-03
rel. contribution = 0.0011 %

left y-axis:

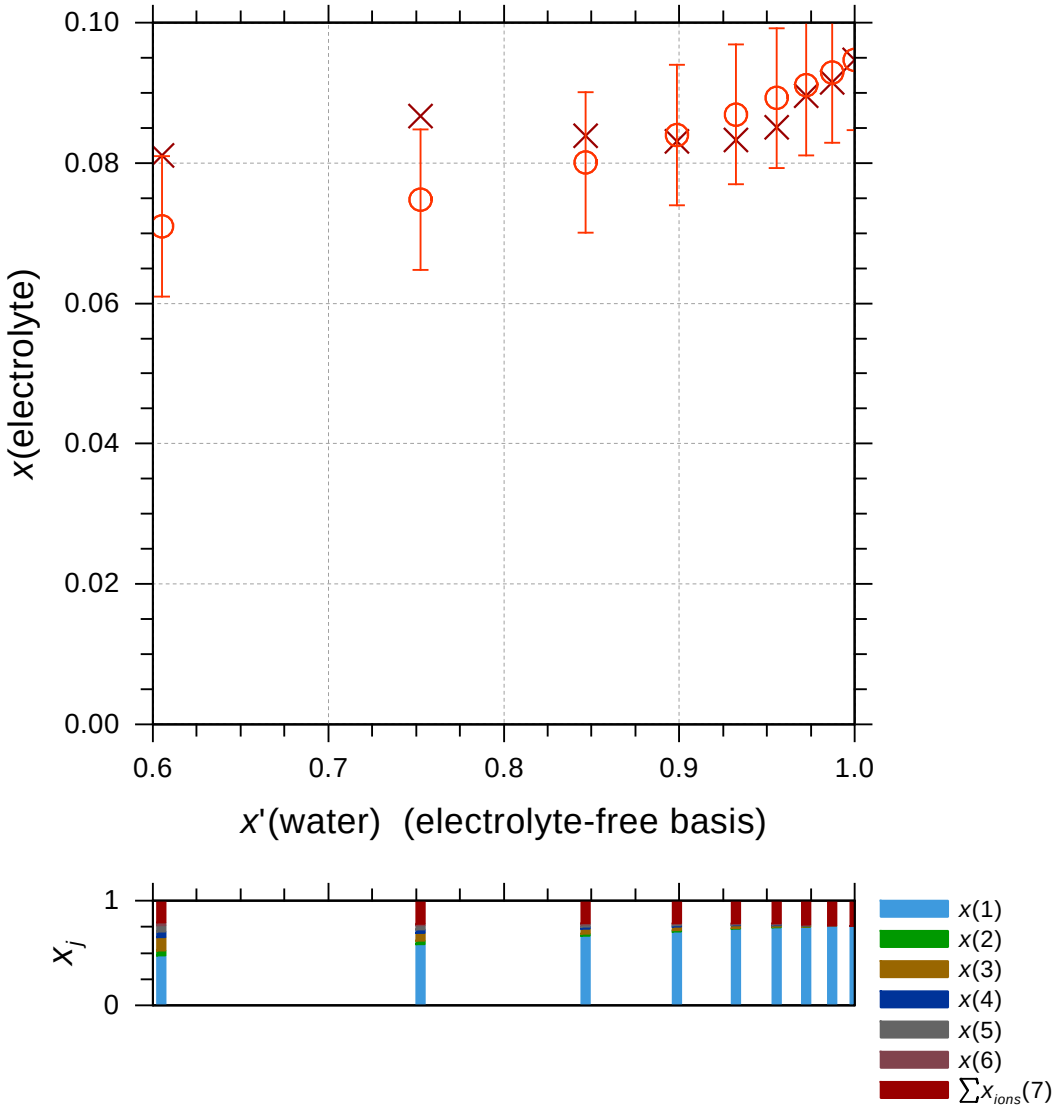
× (NH4)2SO4+DicarboxylicAcidsMixtureM5+Water_SLE-salt_Marcolli

○ AIOMFAC calc. SLE composition

Fig. S0210 (AIOMFAC_output_0285)

H_2O (1) + Malic_acid (2) + Malonic_acid (3) + Maleic_acid (4) + Glutaric_acid (5) + Methylsuccinic_acid (6) + $(NH_4)_2SO_4$

Temperature: 298 K



initial weighting of dataset:

w^{init}(0285) = 1.000

dataset contribution to F_{obj}:

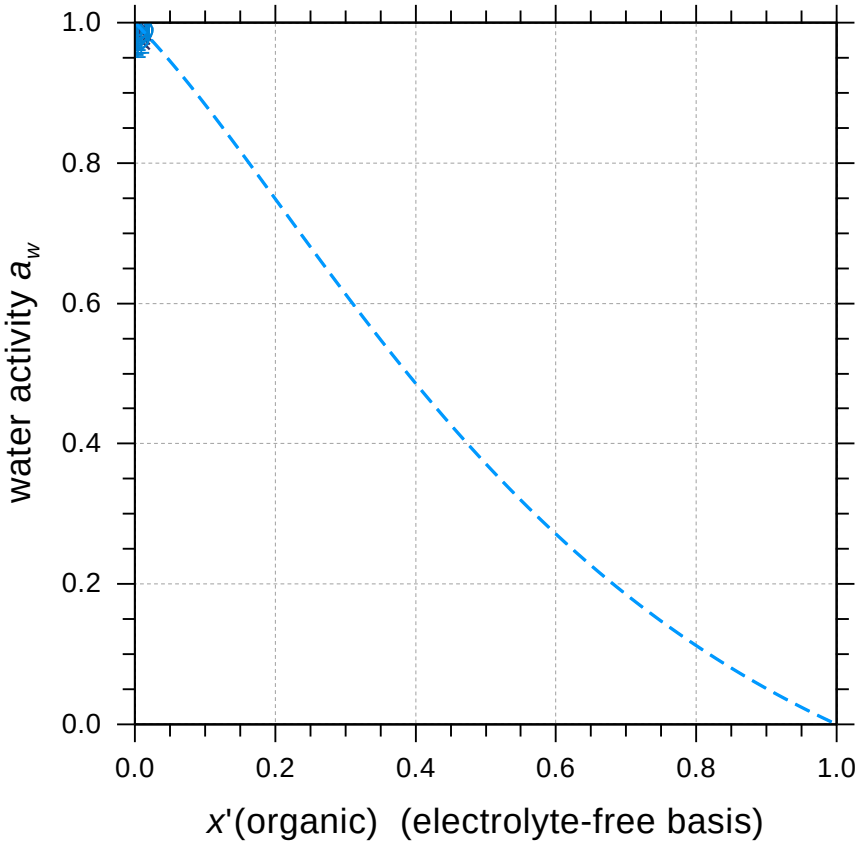
fval(0285) = 3.4521E-02

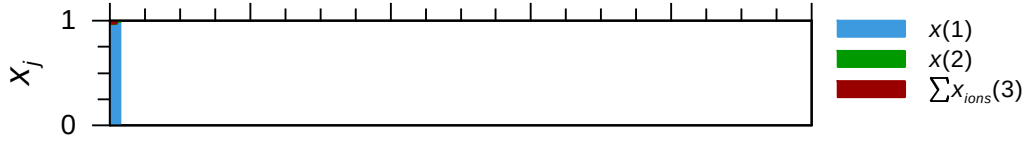
rel. contribution = 0.0164 %

Fig. S0211 (AIOMFAC_output_0377)

H_2O (1) + Oxalic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 293 K



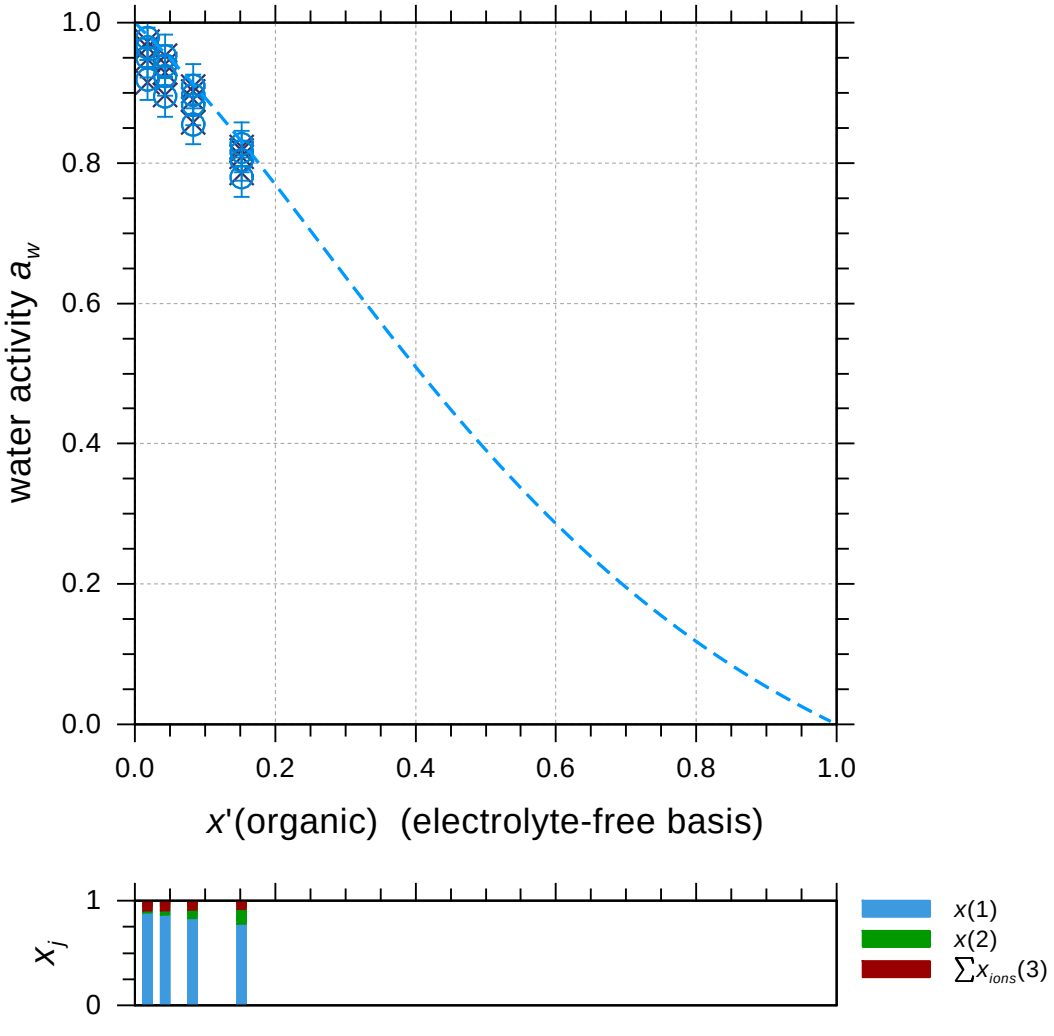


initial weighting of dataset:
$w^{init}(0377)$ = 2.000
dataset contribution to F_{obj}:
fval(0377) = 6.4953E-06
rel. contribution = 0.0000 %

Fig. S0212 (AIOMFAC_output_0378)

H_2O (1) + Malonic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 293 K

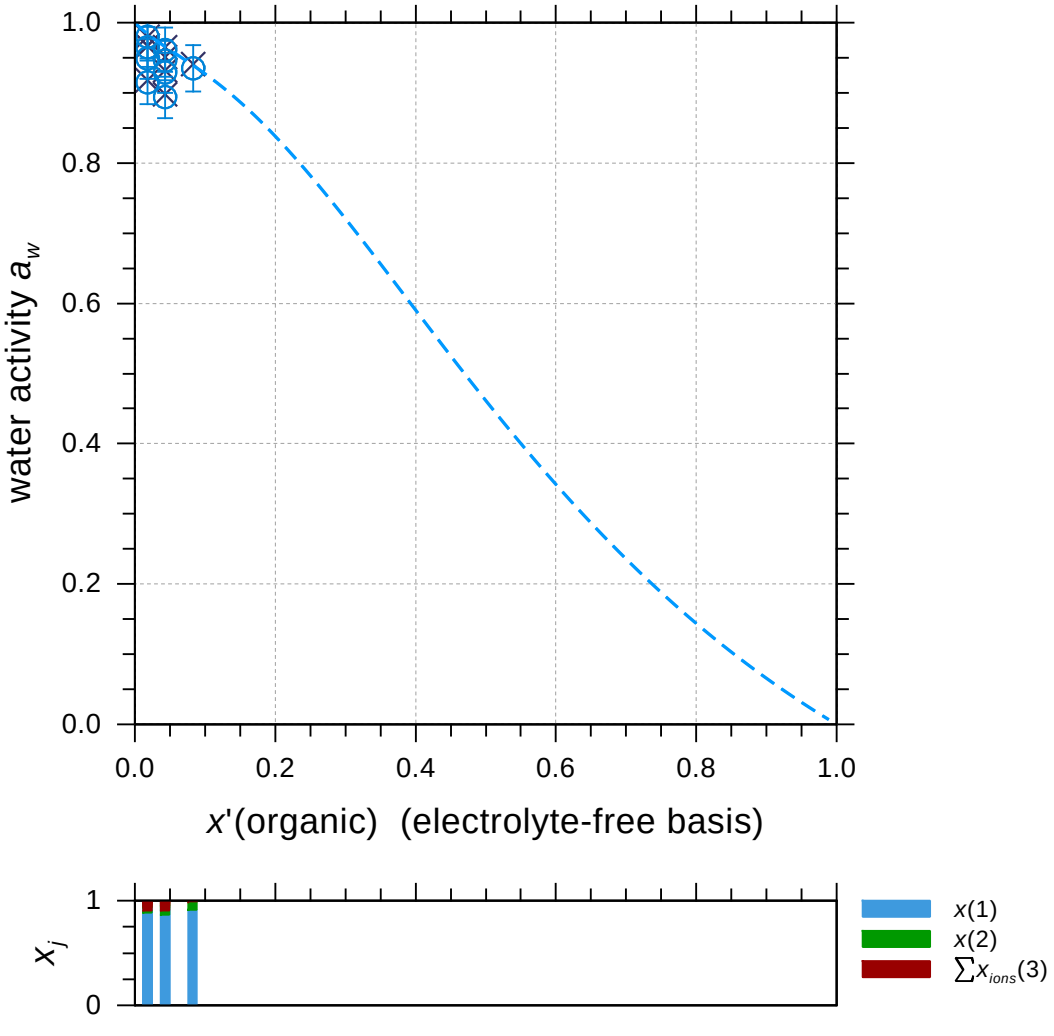


initial weighting of dataset:
$w^{init}(0378)$ = 2.000
dataset contribution to F_{obj}:
fval(0378) = 4.1823E-04
rel. contribution = 0.0002 %

Fig. S0213 (AIOMFAC_output_0379)

H_2O (1) + Glutaric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 293 K

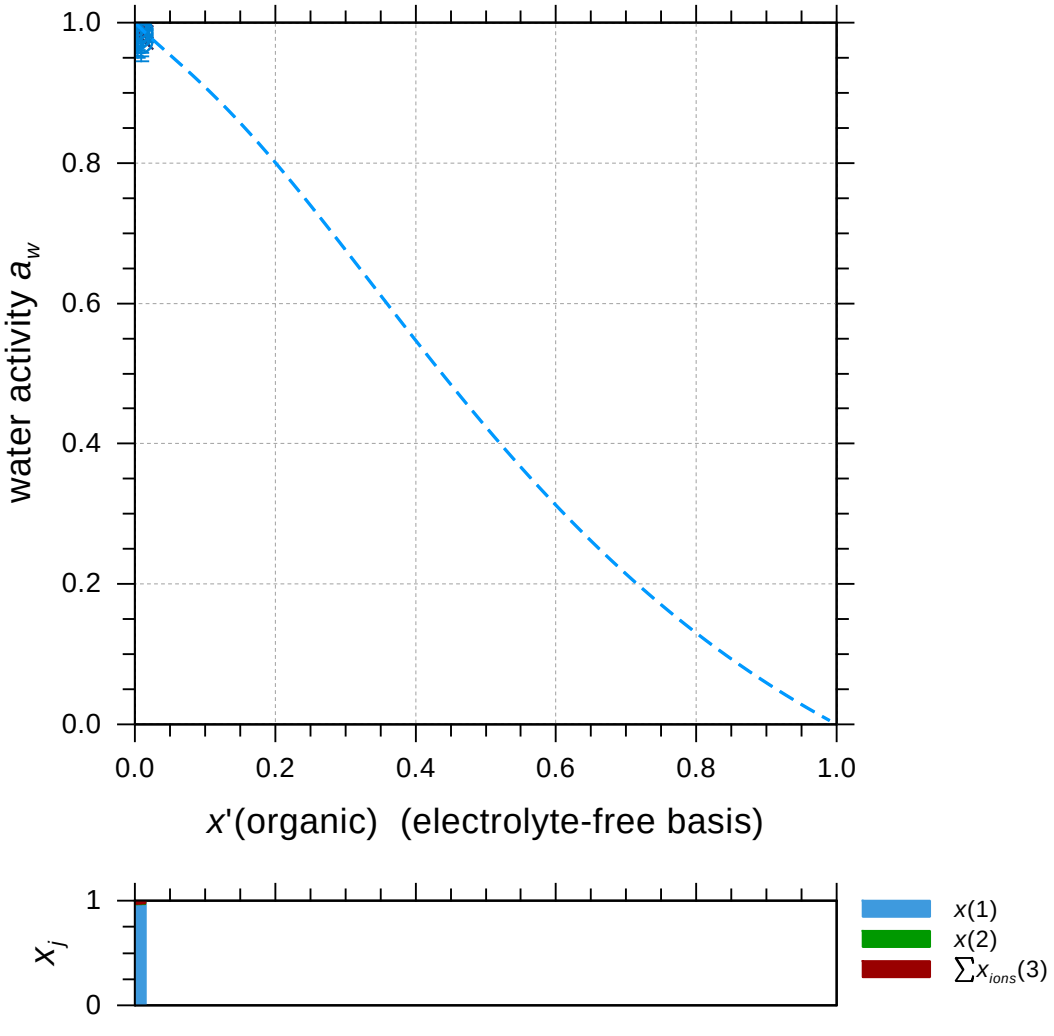


initial weighting of dataset:
$w^{init}(0379)$ = 2.000
dataset contribution to F_{obj}:
fval(0379) = 9.3918E-04
rel. contribution = 0.0004 %

Fig. S0214 (AIOMFAC_output_0380)

H_2O (1) + Succinic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 293 K

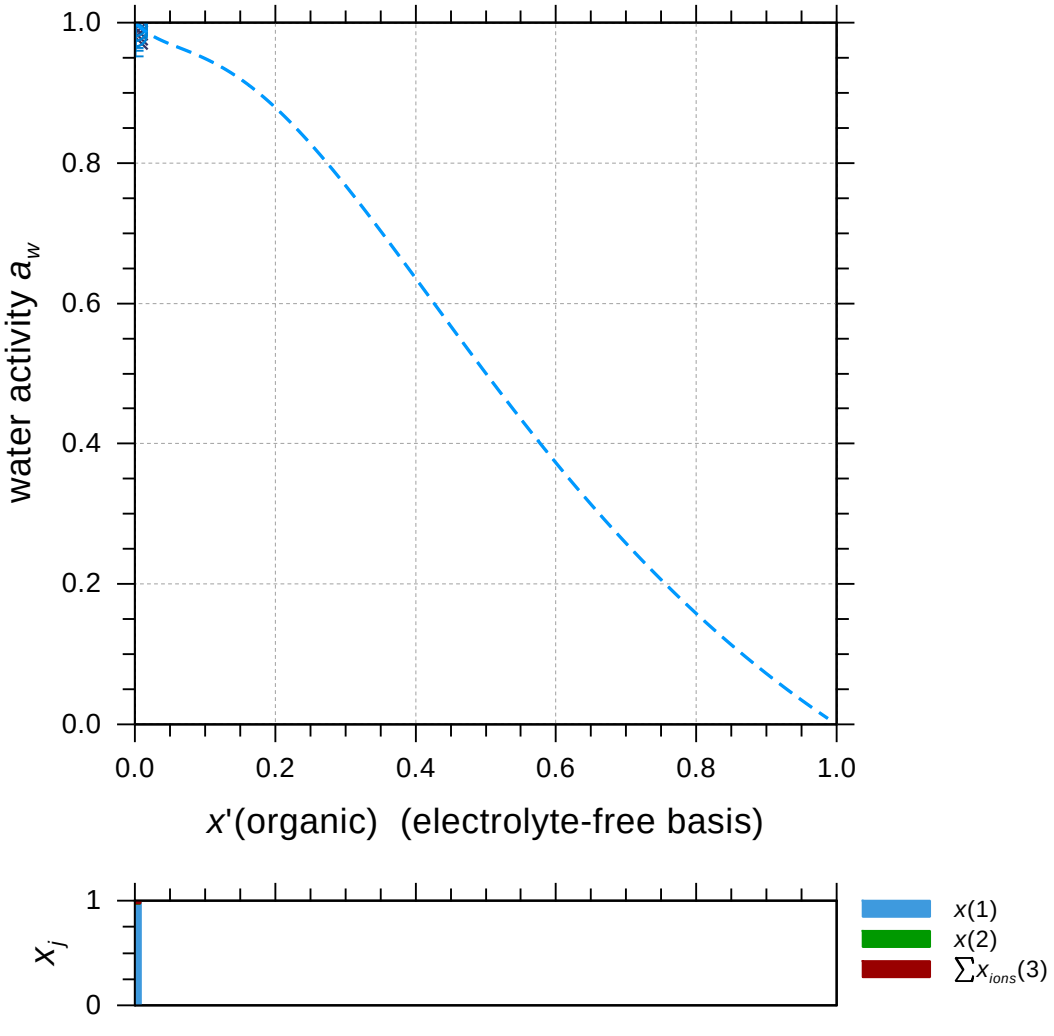


initial weighting of dataset:
$w^{init}(0380)$ = 2.000
dataset contribution to F_{obj}:
fval(0380) = 3.6354E-04
rel. contribution = 0.0002 %

Fig. S0215 (AIOMFAC_output_0381)

H_2O (1) + Adipic_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 293 K

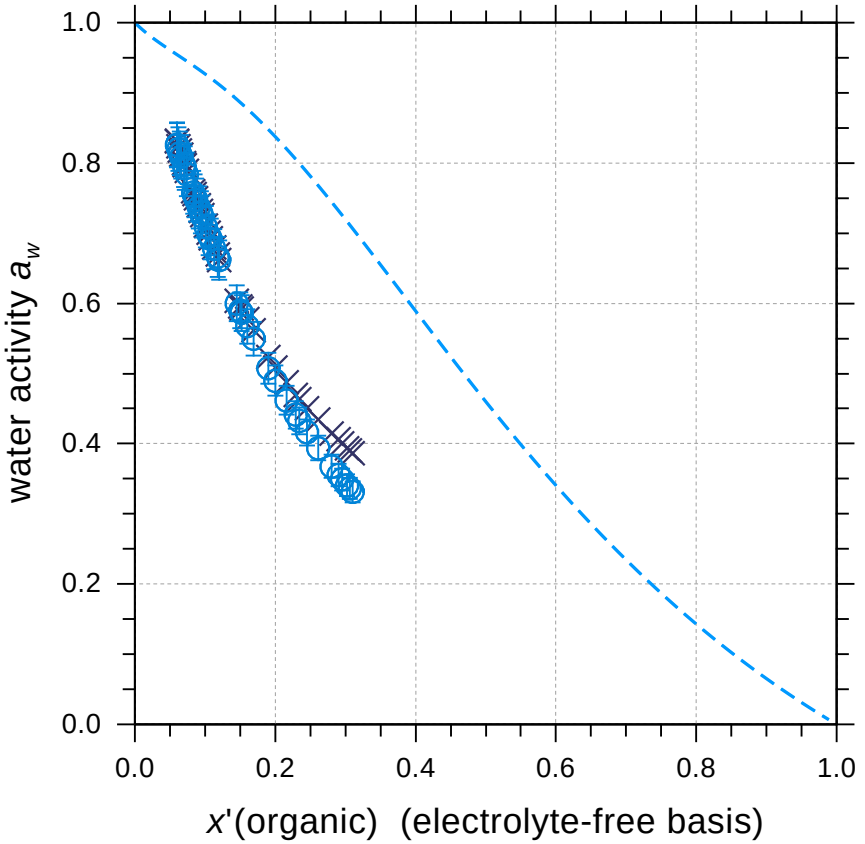


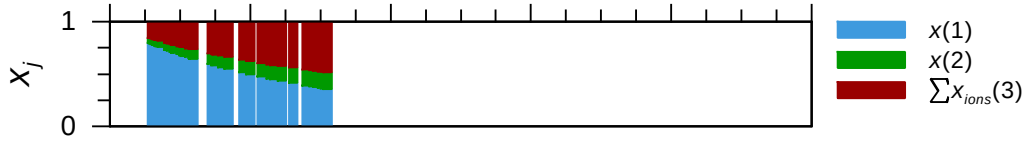
initial weighting of dataset:
$w^{init}(0381)$ = 2.000
dataset contribution to F_{obj}:
fval(0381) = 1.0514E-04
rel. contribution = 0.0000 %

Fig. S0216 (AIOMFAC_output_0960)

H_2O (1) + Glutaric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 291 K



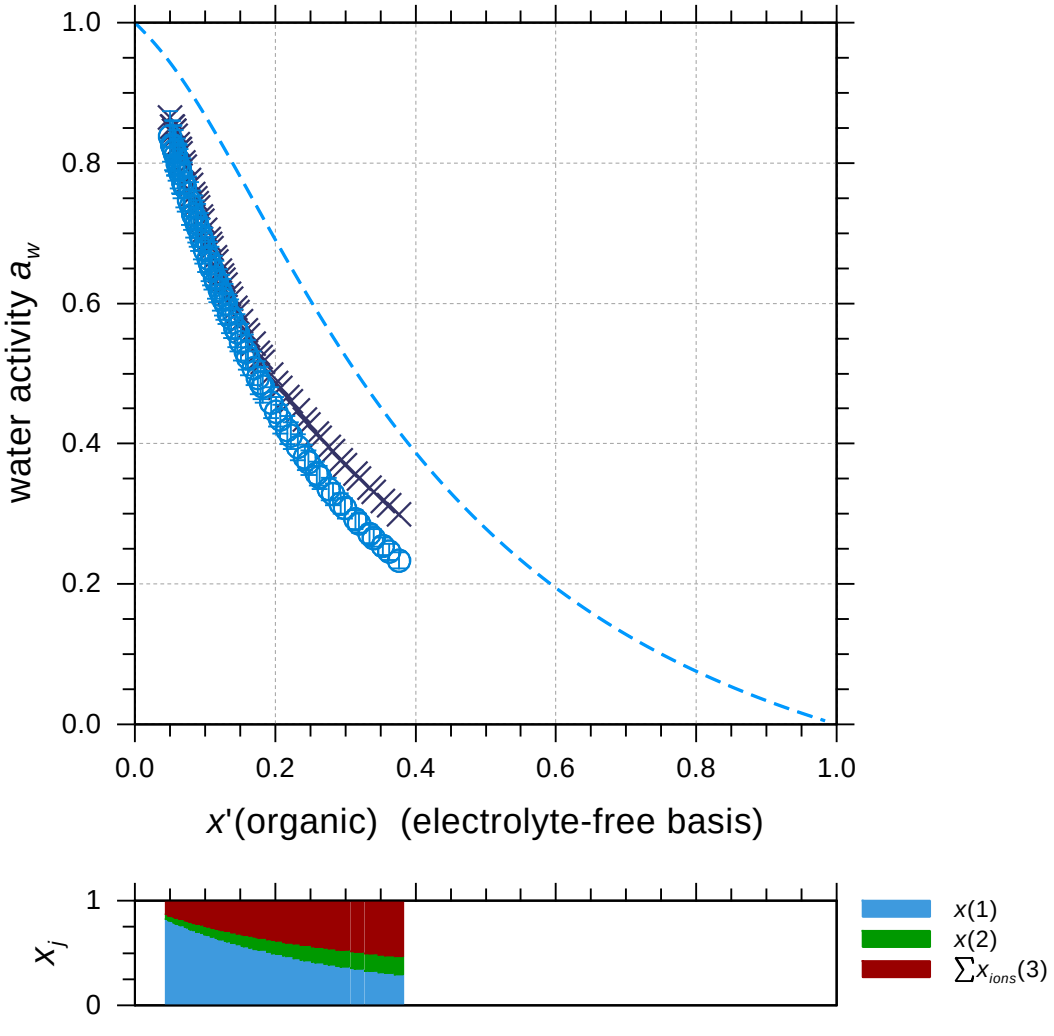


initial weighting of dataset:
$w^{init}(0960)$ = 1.000
dataset contribution to F_{obj}:
fval(0960) = 3.1627E-02
rel. contribution = 0.0150 %

Fig. S0217 (AIOMFAC_output_0961)

H_2O (1) + Citric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 291 K

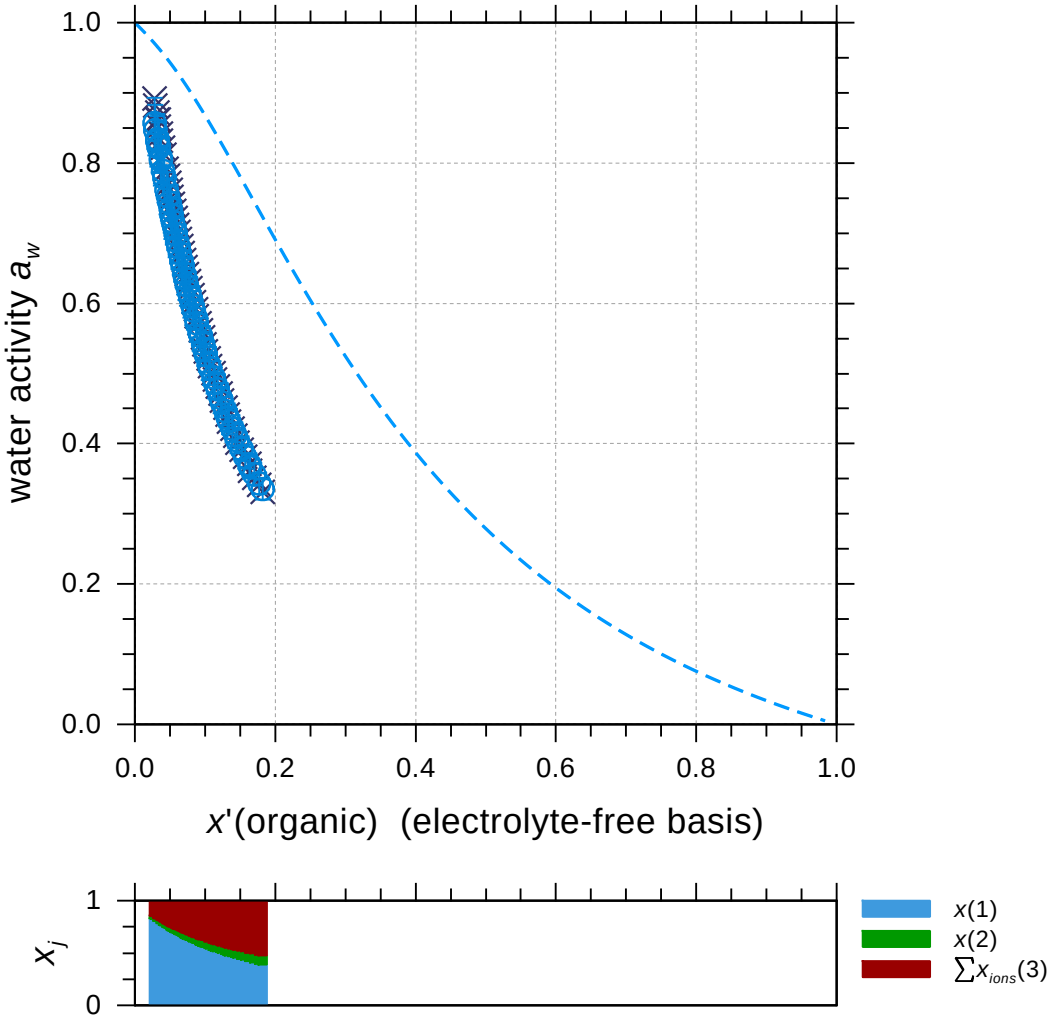


initial weighting of dataset:
$w^{init}(0961)$ = 1.000
dataset contribution to F_{obj}:
fval(0961) = 8.7440E-02
rel. contribution = 0.0416 %

Fig. S0218 (AIOMFAC_output_0962)

H_2O (1) + Citric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 291 K

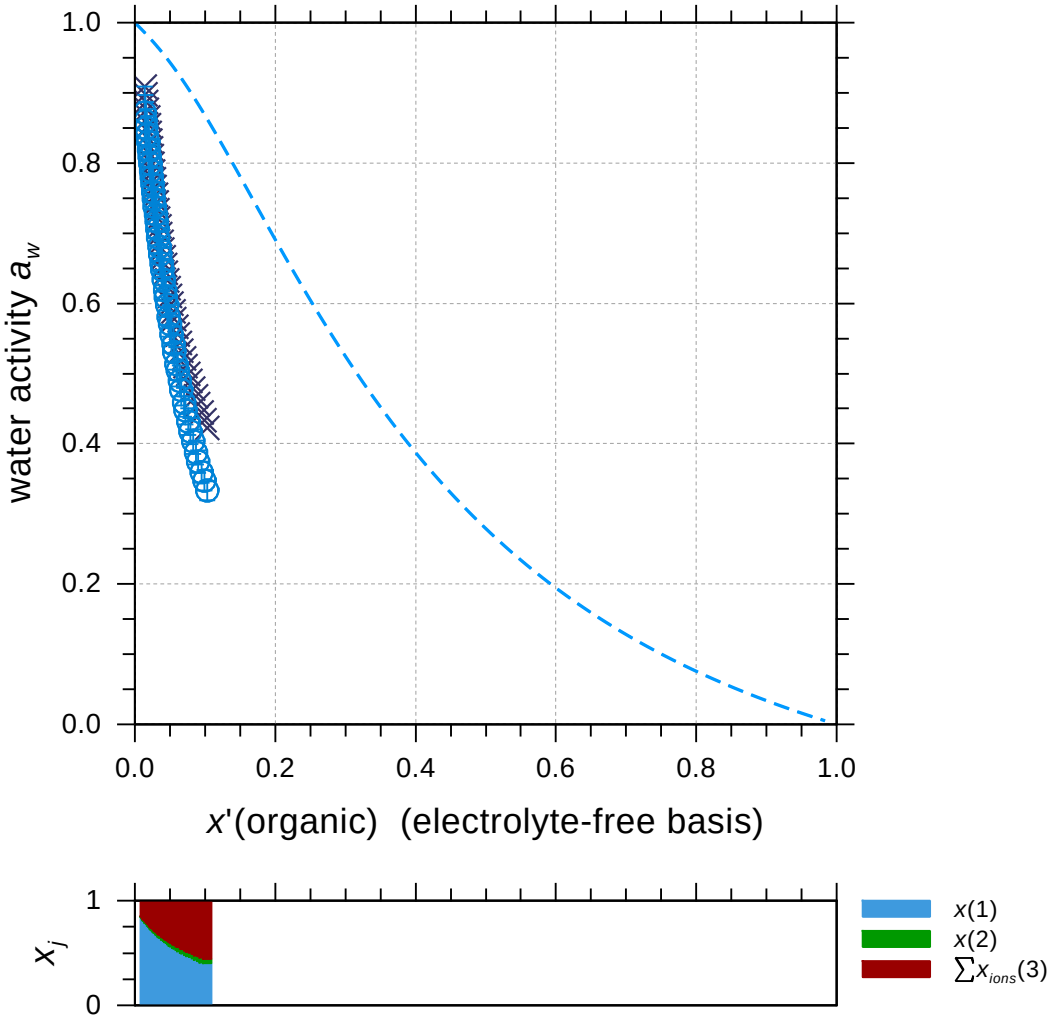


initial weighting of dataset:
$w^{init}(0962)$ = 1.000
dataset contribution to F_{obj}:
fval(0962) = 6.1875E-03
rel. contribution = 0.0029 %

Fig. S0219 (AIOMFAC_output_0963)

H_2O (1) + Citric_acid (2) + $(NH_4)_2SO_4$ (3)

Temperature: 291 K



initial weighting of dataset:
$w^{init}(0963)$ = 1.000
dataset contribution to F_{obj}:
fval(0963) = 8.0265E-02
rel. contribution = 0.0382 %

left y-axis:

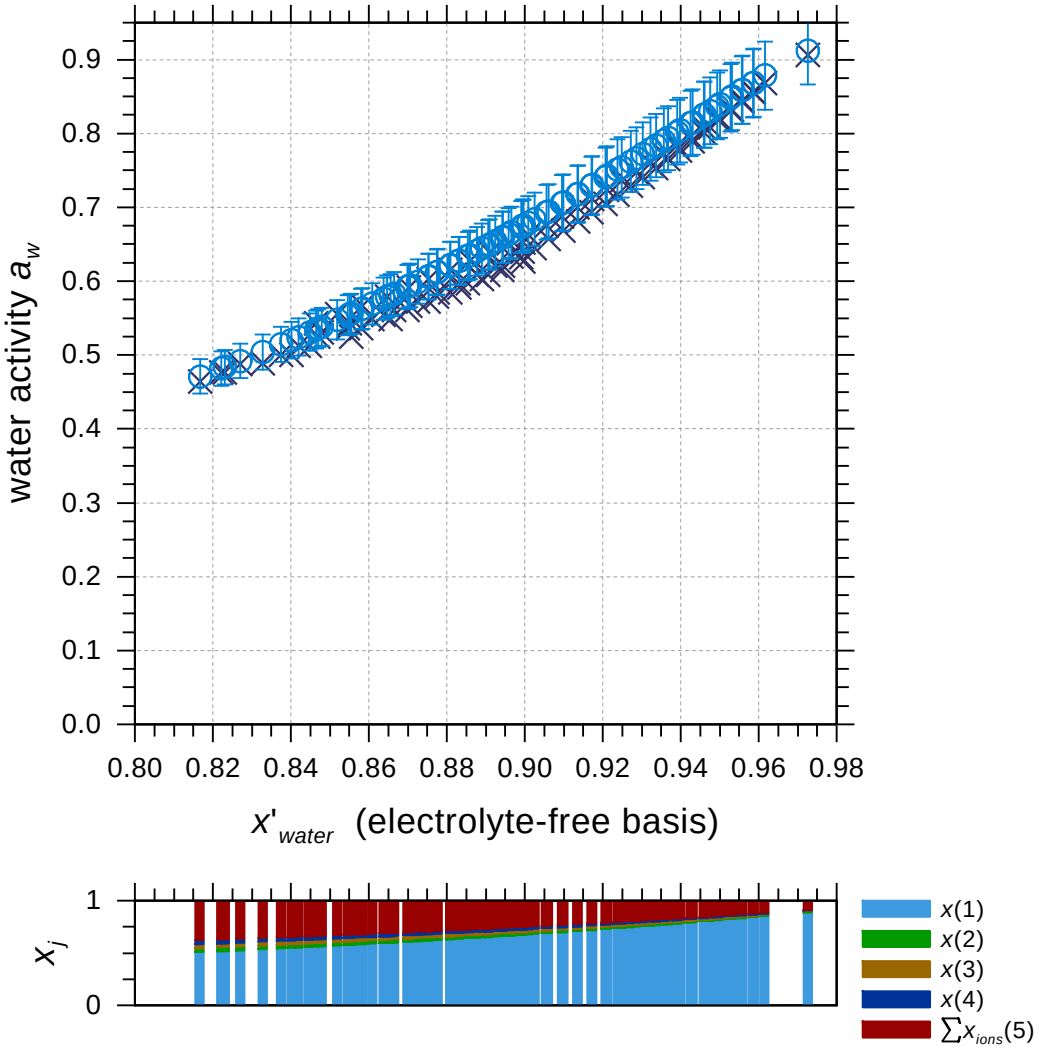
× C6+AS+Water_aw_data

○ AIOMFAC water activity a_w

Fig. S0220 (AIOMFAC_output_1059)

H_2O (1) + 2-Methylglutaric_acid (2) + 3-Methylglutaric_acid (3) + 2,2-Dimethylsuccinic_acid (4) + $(NH_4)_2SO_4$ (5)

Temperature range: 291 -- 293 K

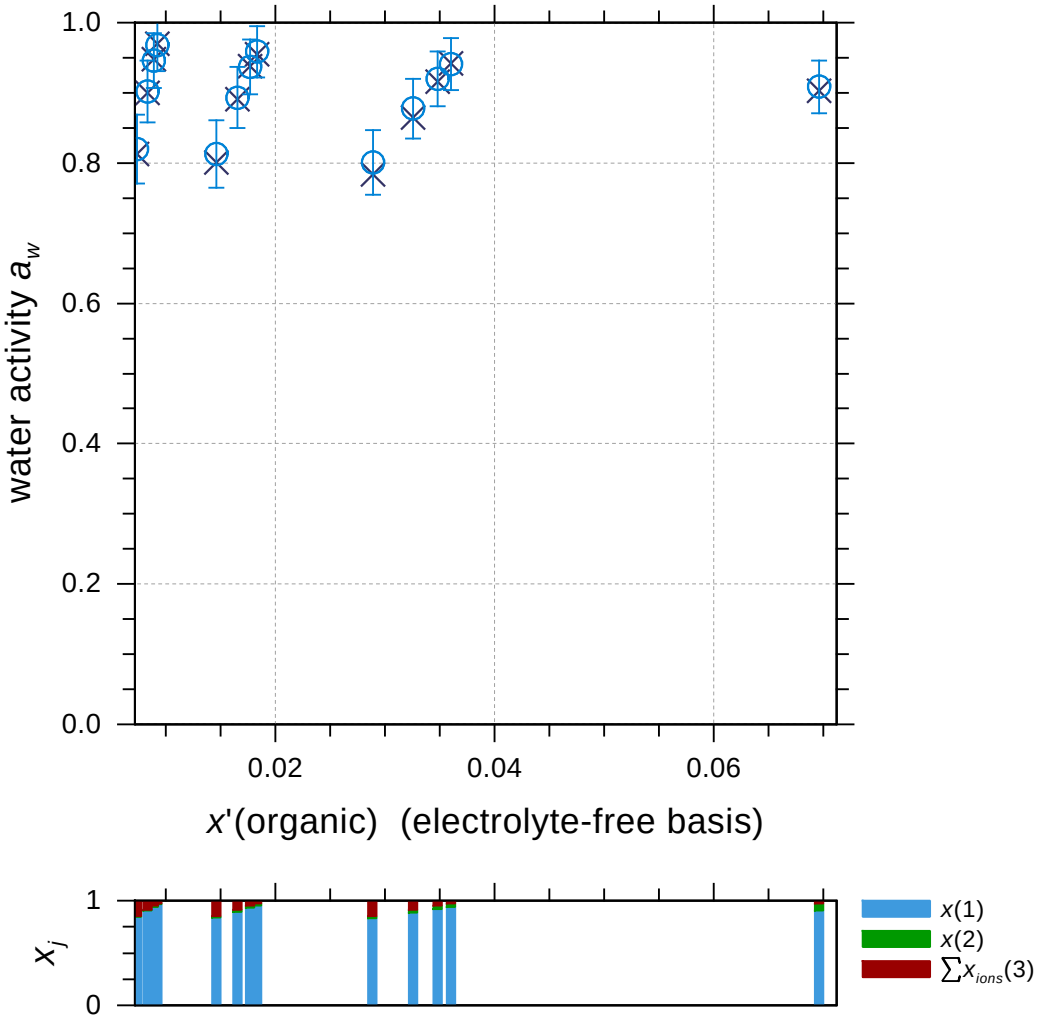


initial weighting of dataset:
$w^{init}(1059)$ = 1.000
dataset contribution to F_{obj}:
fval(1059) = 1.4081E-02
rel. contribution = 0.0067 %

Fig. S0221 (AIOMFAC_output_0968)

H_2O (1) + Maleic_acid (2) + $Ca(NO_3)_2$ (3)

Temperature: 293 K



initial weighting of dataset:
$w^{init}(0968)$ = 2.000
dataset contribution to F_{obj}:
fval(0968) = 1.4880E-03
rel. contribution = 0.0007 %

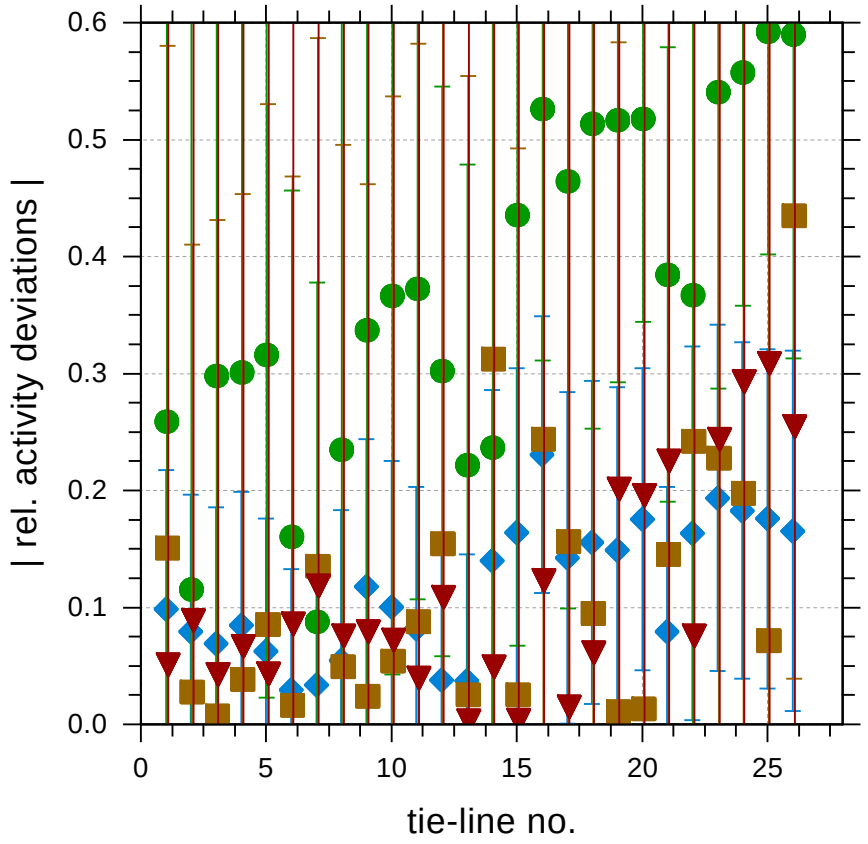
Fig. S0222 (AIOMFAC_output_0311)

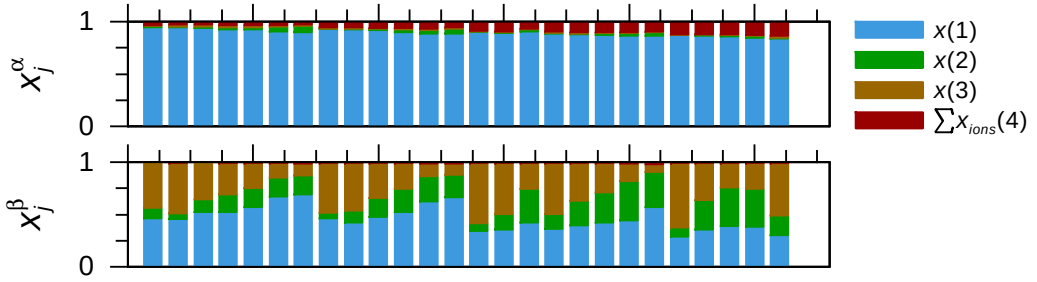
H_2O (1) + Propanoic_acid (2) + 1-Butanol (3) + $CaCl_2$ (4)

Temperature: 303 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



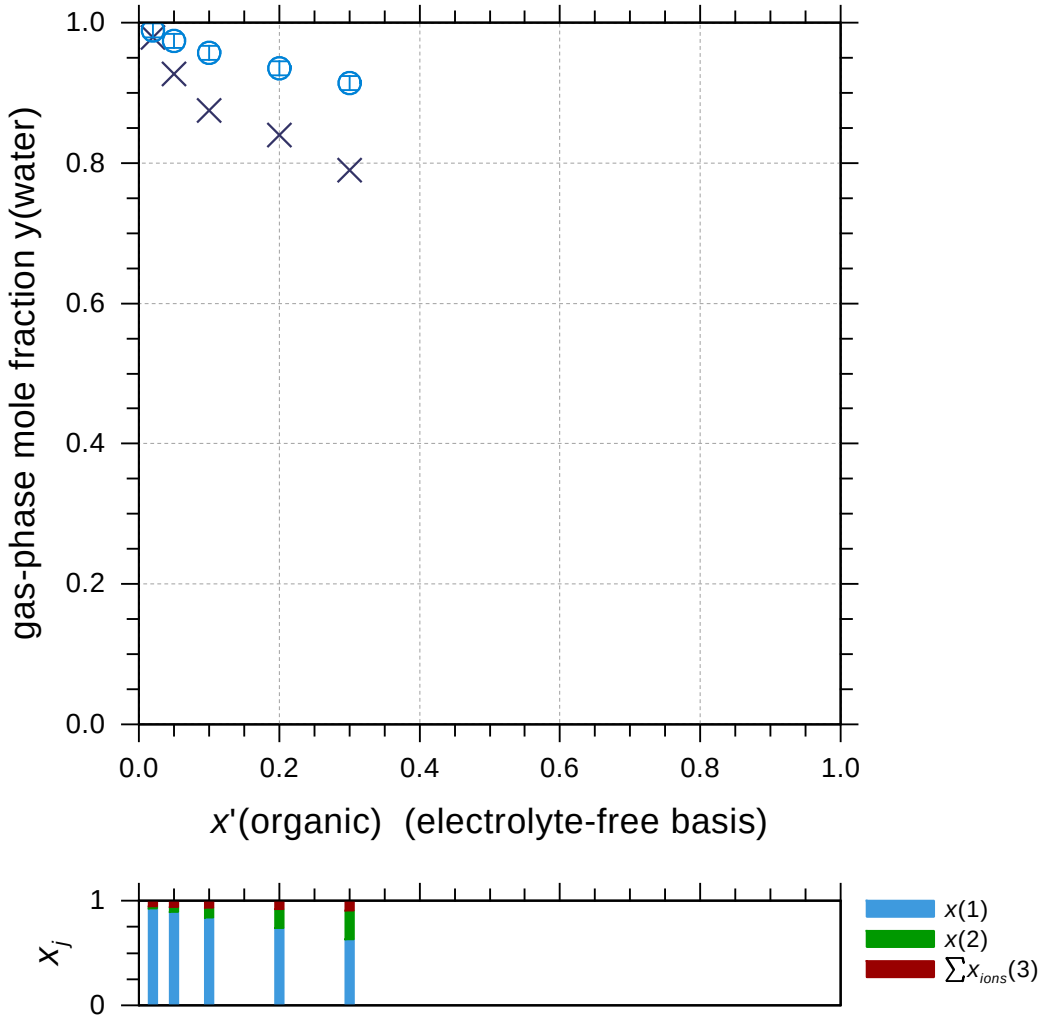


initial weighting of dataset:
w^{init}(0311) = 1.000
dataset contribution to F_{obj}:
fval(0311) = 1.0965E+00
rel. contribution = 0.5214 %

Fig. S0223 (AIOMFAC_output_0332)

H_2O (1) + Propanoic_acid (2) + $CaCl_2$ (3)

Temperature: 333 K

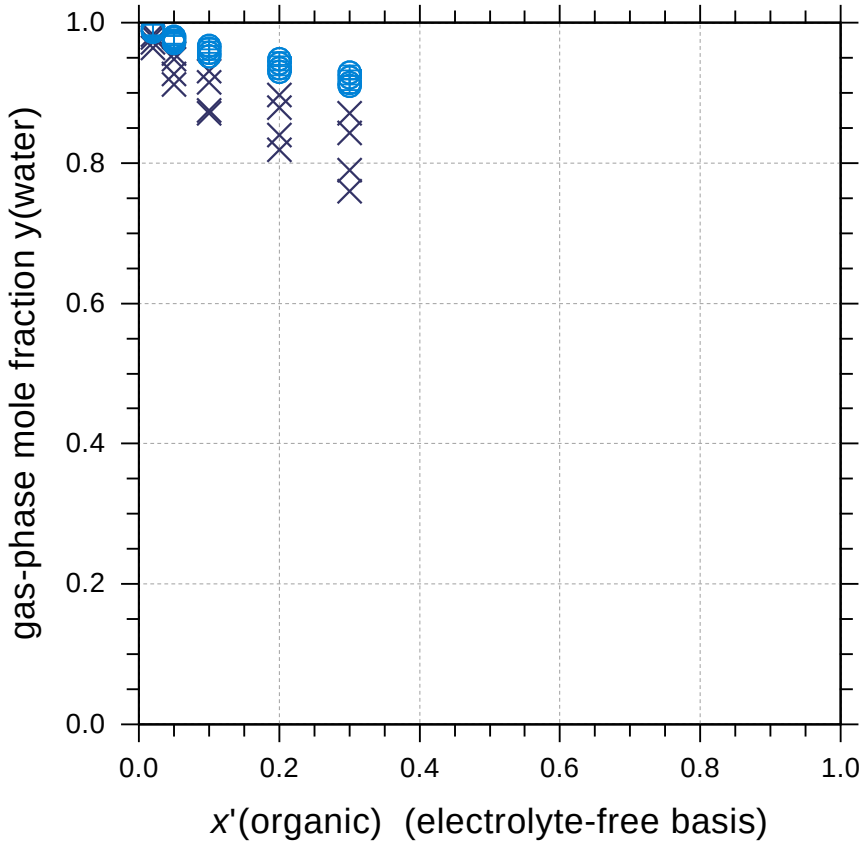


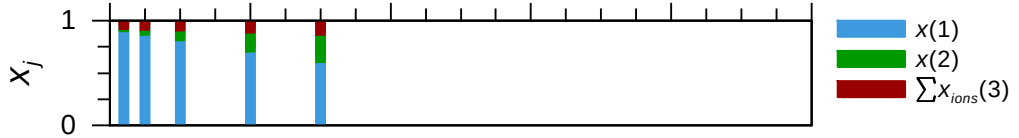
initial weighting of dataset:
$w^{init}(0332)$ = 0.500
dataset contribution to F_{obj}:
fval(0332) = 2.3644E-02
rel. contribution = 0.0112 %

Fig. S0224 (AIOMFAC_output_0334)

H_2O (1) + Propanoic_acid (2) + $CaCl_2$ (3)

Temperature: 333 K





left y-axis:

× CaCl2+PropanoicAcid+Water_VLE_Banat2003

○ AIOMFAC gas-phase composition y(water)

initial weighting of dataset:

w^{init}(0334) = 0.500

dataset contribution to F_{obj}:

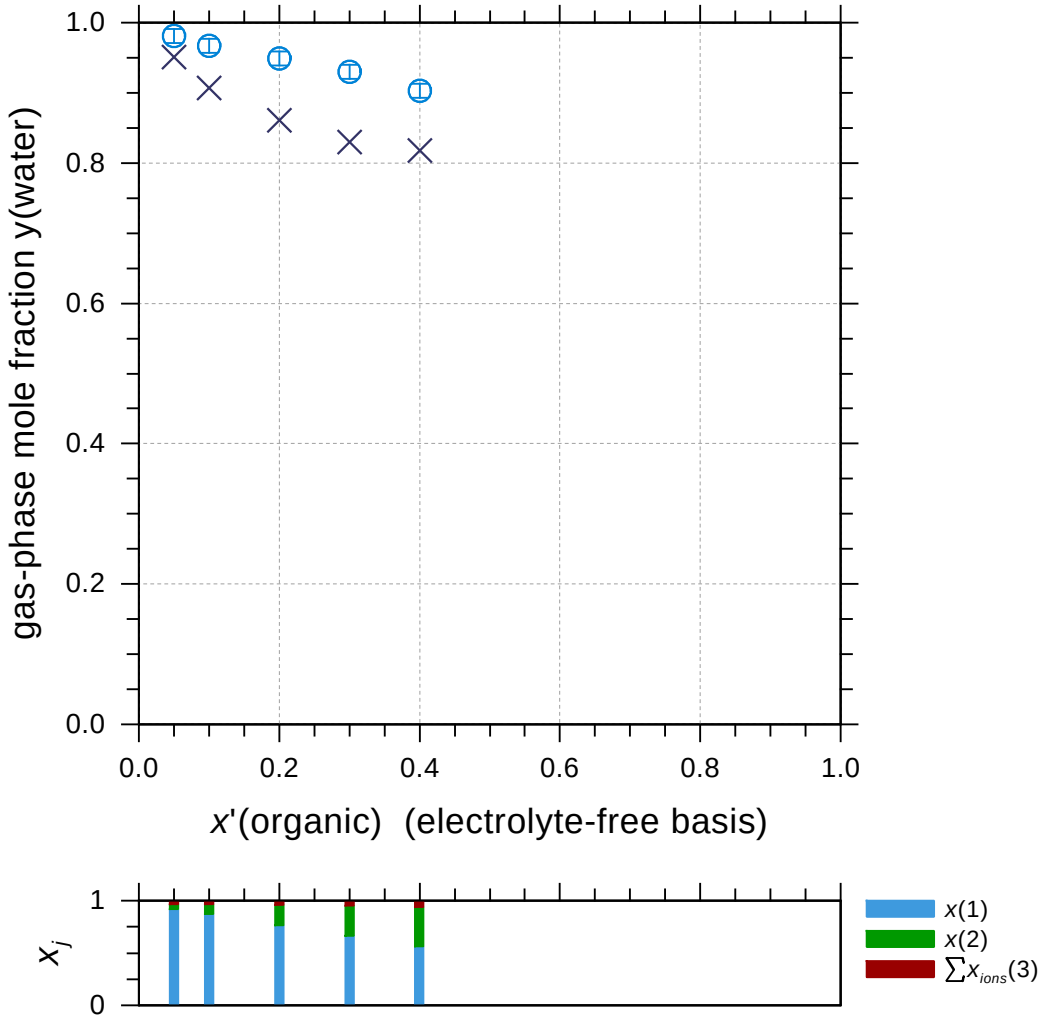
fval(0334) = 3.5816E-02

rel. contribution = 0.0170 %

Fig. S0225 (AIOMFAC_output_0342)

H_2O (1) + Propanoic_acid (2) + $CaCl_2$ (3)

Temperature: 313 K

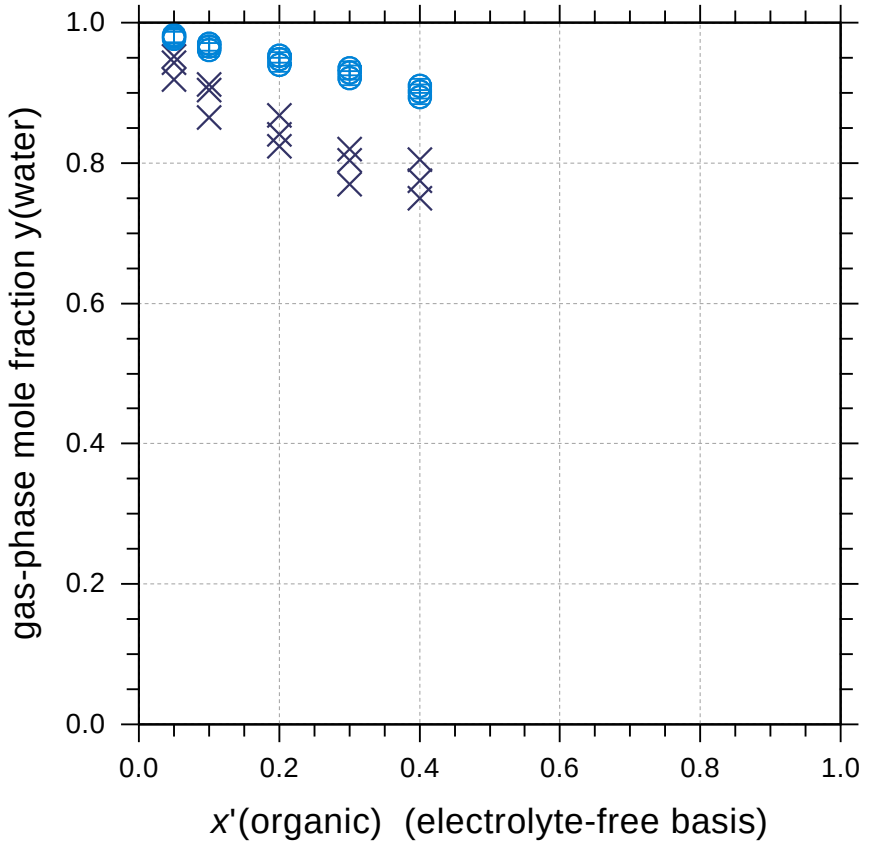


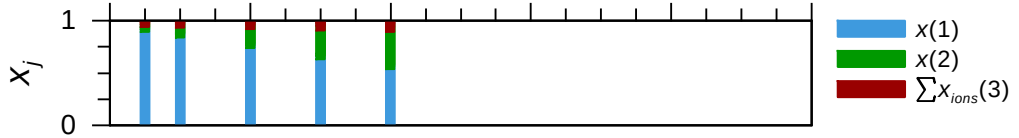
initial weighting of dataset:
$w^{init}(0342)$ = 0.500
dataset contribution to F_{obj}:
fval(0342) = 2.0064E-02
rel. contribution = 0.0095 %

Fig. S0226 (AIOMFAC_output_0343)

H_2O (1) + Propanoic_acid (2) + $CaCl_2$ (3)

Temperature: 323 K





left y-axis:

× CaCl2+PropanoicAcid+Water_VLE_Banat_323K

○ AIOMFAC gas-phase composition y(water)

initial weighting of dataset:

$w^{init}(0343)$ = 0.500

dataset contribution to F_{obj}:

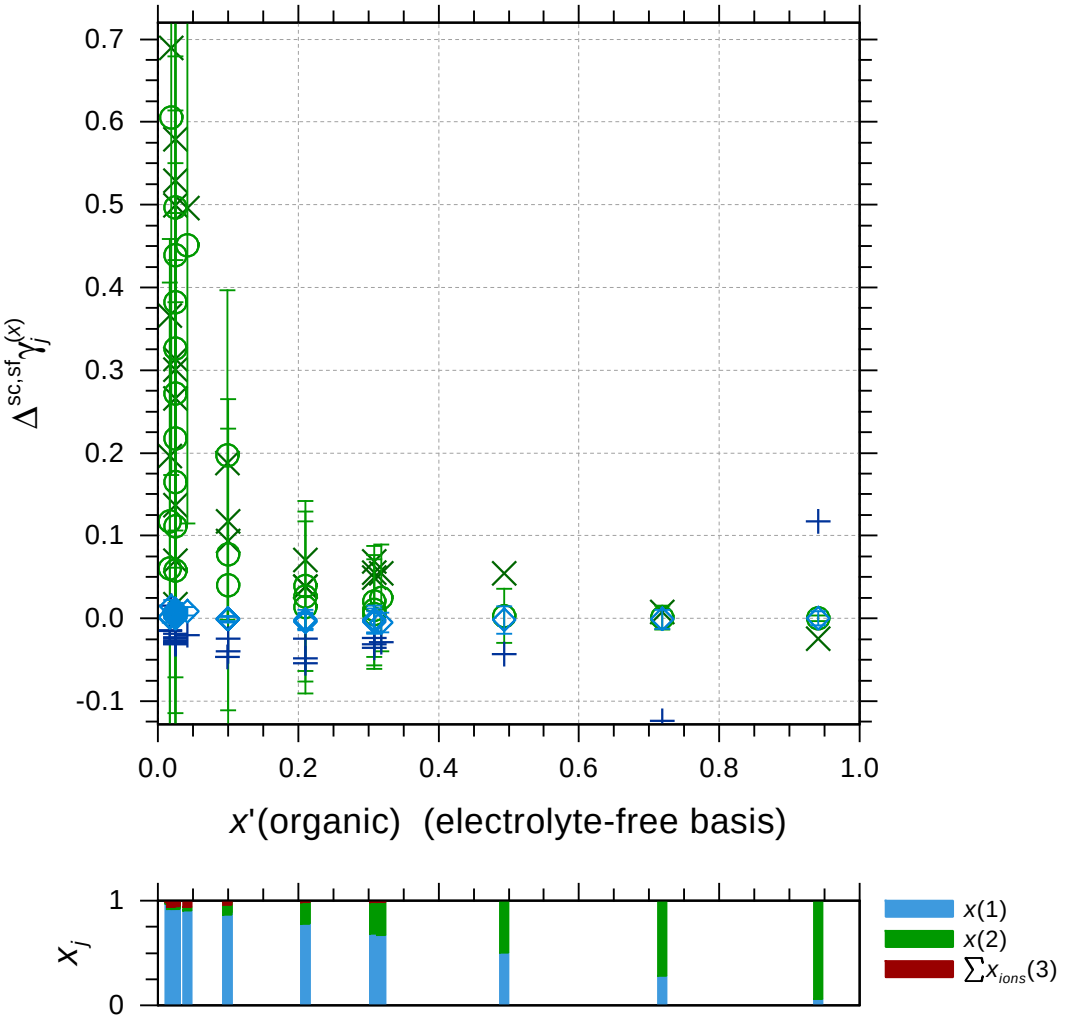
fval(0343) = 7.6859E-02

rel. contribution = 0.0365 %

Fig. S0227 (AIOMFAC_output_0329)

H_2O (1) + Acetic_acid (2) + K_2SO_4 (3)

Temperature range: 373 -- 388 K

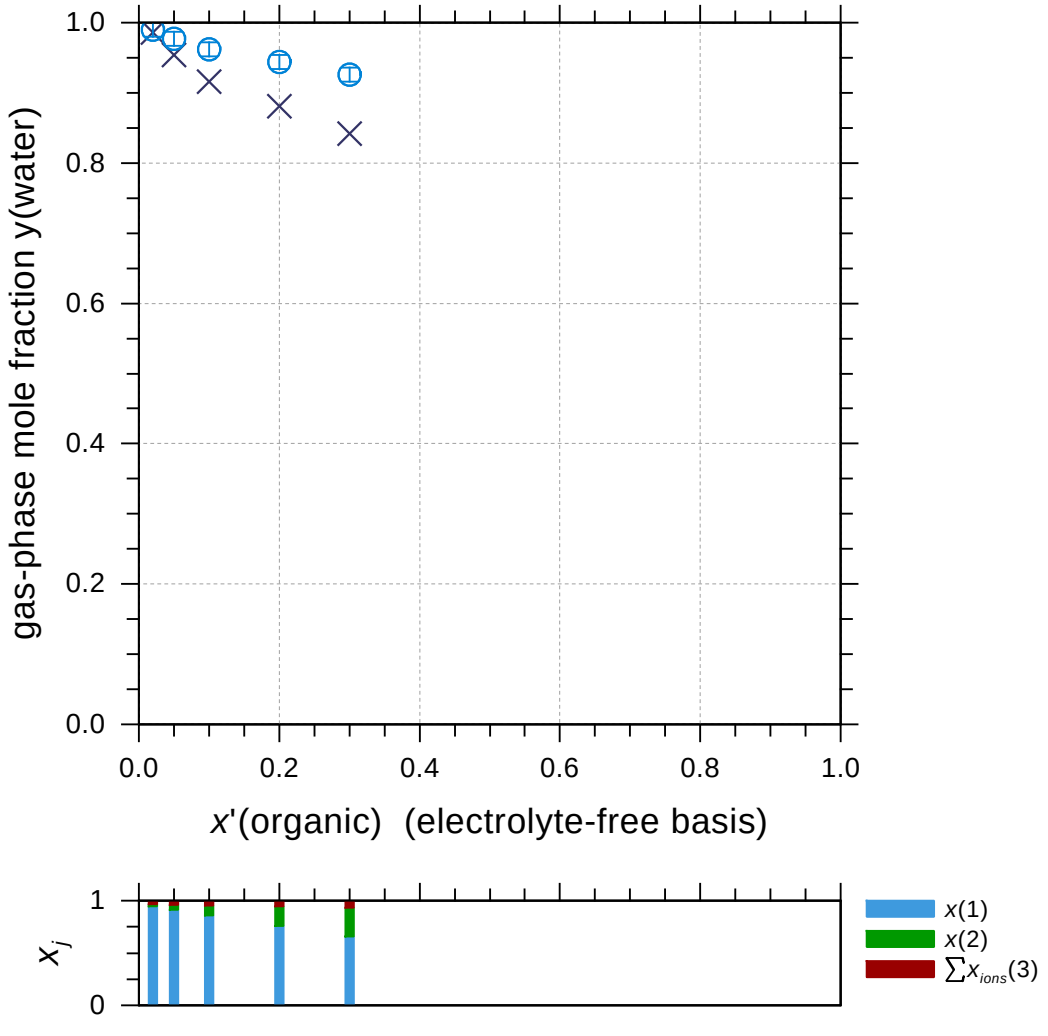


initial weighting of dataset:
$w^{init}(0329)$ = 0.500
dataset contribution to F_{obj}:
fval(0329) = 1.9788E-02
rel. contribution = 0.0094 %

Fig. S0228 (AIOMFAC_output_0336)

H_2O (1) + Propanoic_acid (2) + KBr (3)

Temperature: 333 K

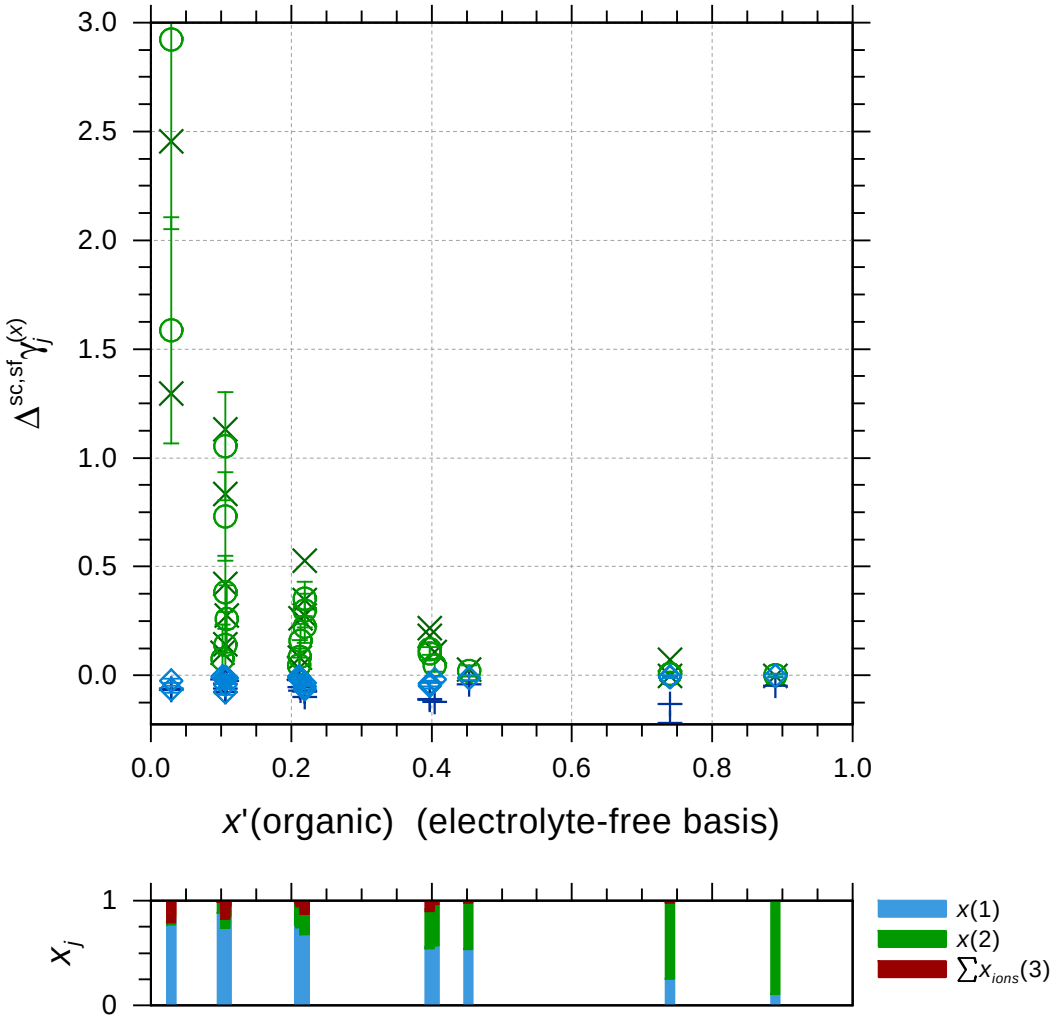


initial weighting of dataset:
$w^{init}(0336)$ = 0.500
dataset contribution to F_{obj}:
fval(0336) = 8.8159E-03
rel. contribution = 0.0042 %

Fig. S0229 (AIOMFAC_output_0327)

H_2O (1) + Acetic_acid (2) + KCl (3)

Temperature range: 374 -- 386 K

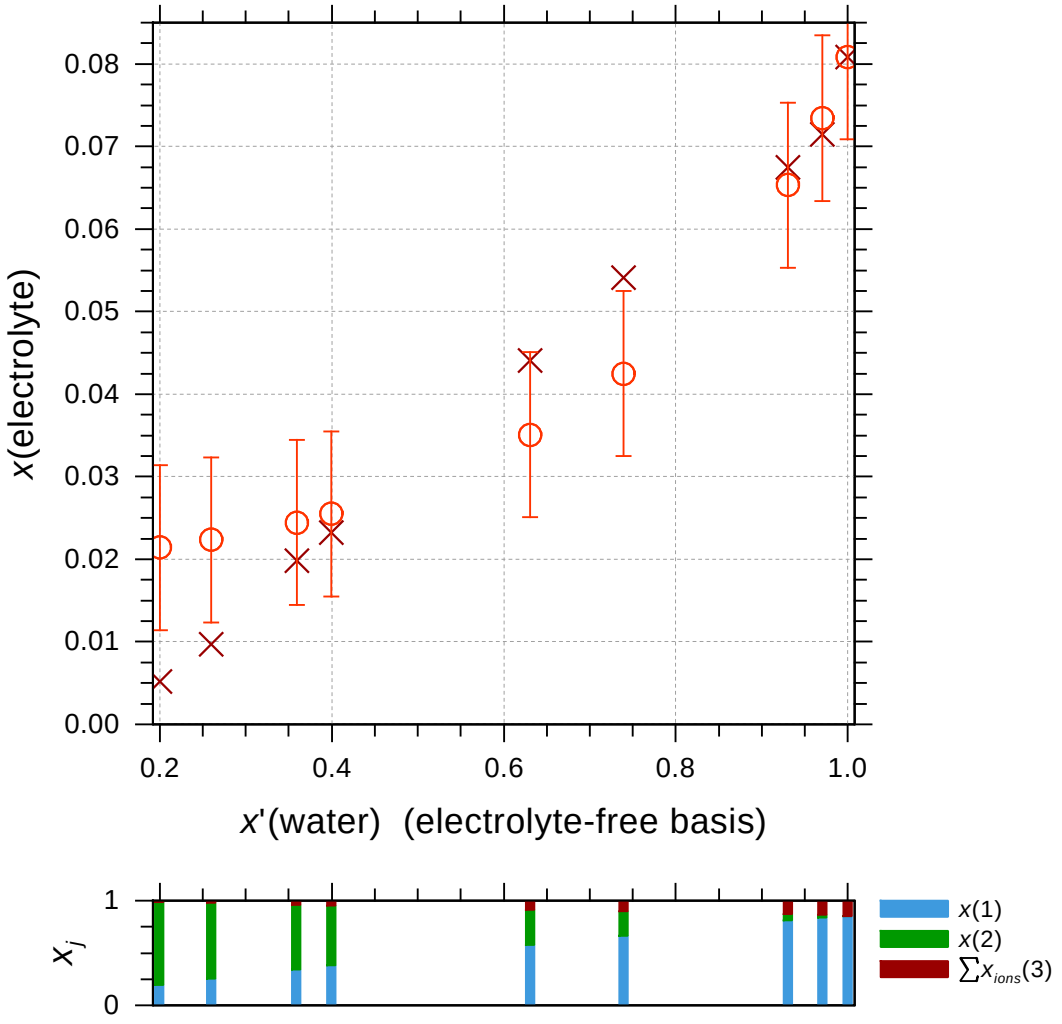


initial weighting of dataset:
$w^{init}(0327)$ = 0.500
dataset contribution to F_{obj}:
fval(0327) = 3.1909E-02
rel. contribution = 0.0152 %

Fig. S0230 (AIOMFAC_output_0330)

H_2O (1) + Acetic_acid (2) + KCl (3)

Temperature: 303 K

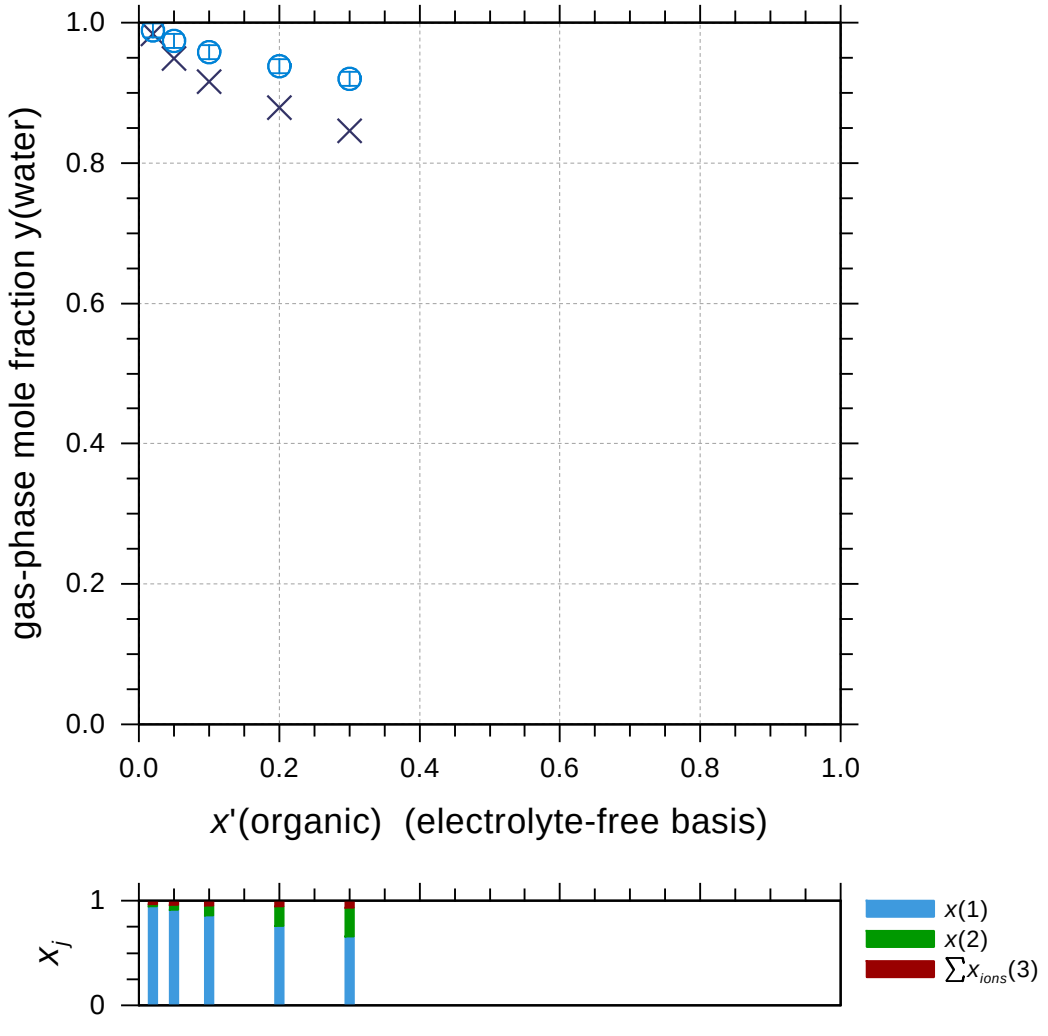


initial weighting of dataset:
$w^{init}(0330)$ = 0.500
dataset contribution to F_{obj}:
fval(0330) = 8.2587E-01
rel. contribution = 0.3927 %

Fig. S0231 (AIOMFAC_output_0335)

H_2O (1) + Propanoic_acid (2) + KCl (3)

Temperature: 333 K

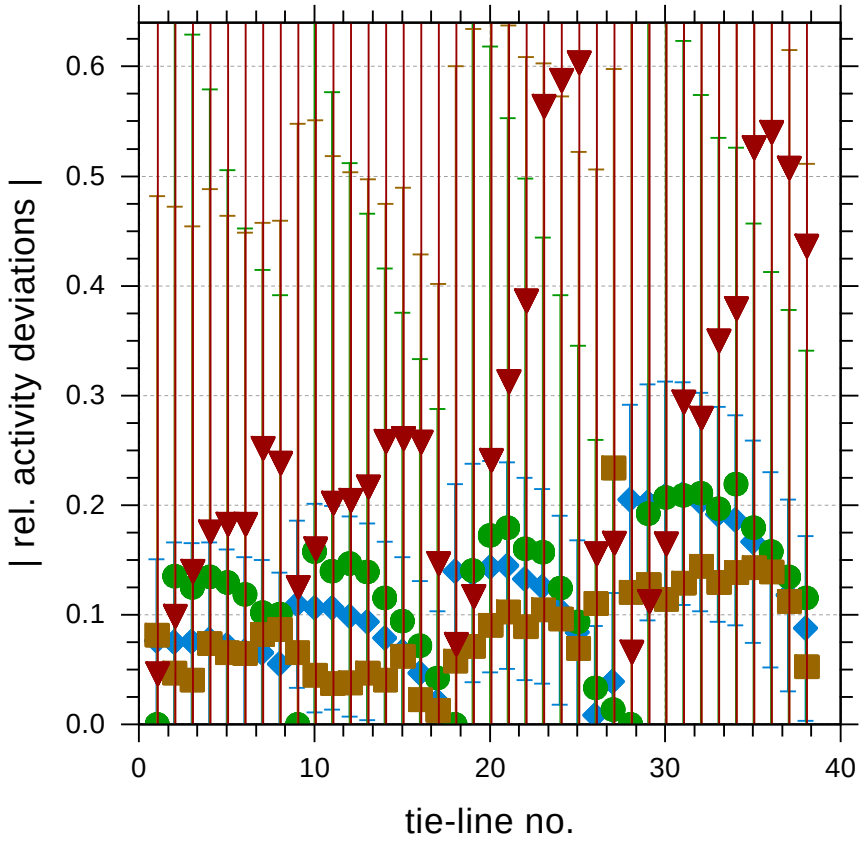


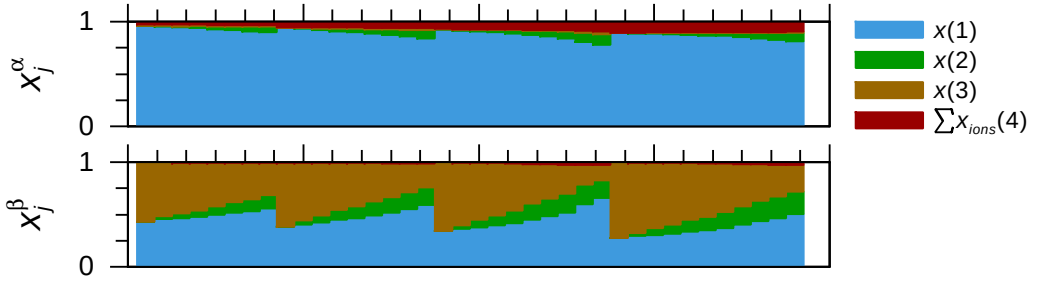
initial weighting of dataset:
$w^{init}(0335)$ = 0.500
dataset contribution to F_{obj}:
fval(0335) = 7.2956E-03
rel. contribution = 0.0035 %

Fig. S0232 (AIOMFAC_output_0933)

H_2O (1) + Acetic_acid (2) + 1-Butanol (3) + KCl (4)

Temperature: 298 K



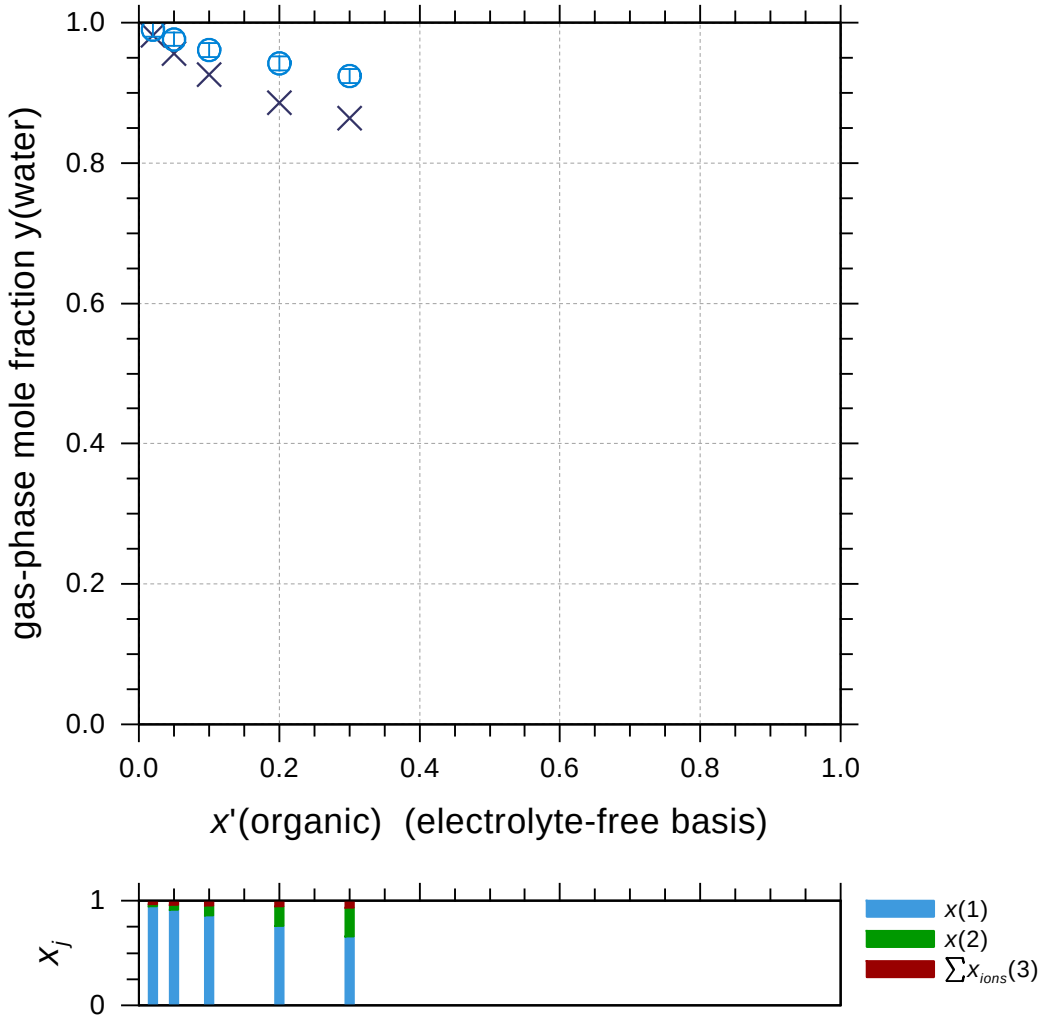


initial weighting of dataset:
$w^{init}(0933)$ = 1.000
dataset contribution to F_{obj}:
fval(0933) = 6.8425E-01
rel. contribution = 0.3254 %

Fig. S0233 (AIOMFAC_output_0337)

H_2O (1) + Propanoic_acid (2) + KNO_3 (3)

Temperature: 333 K

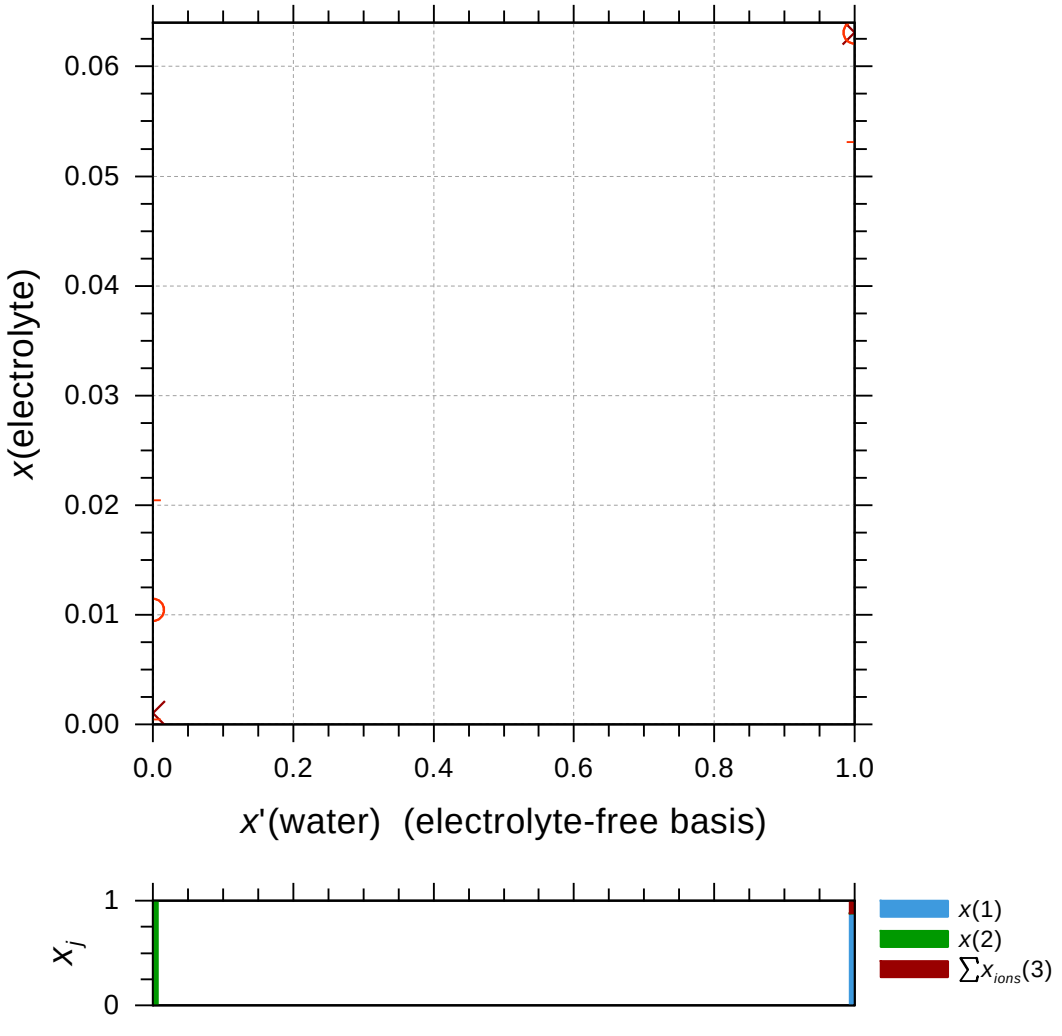


initial weighting of dataset:
$w^{init}(0337)$ = 0.500
dataset contribution to F_{obj}:
fval(0337) = 5.2603E-03
rel. contribution = 0.0025 %

Fig. S0234 (AIOMFAC_output_0941)

H_2O (1) + Acetic_acid (2) + KNO_3 (3)

Temperature: 298 K

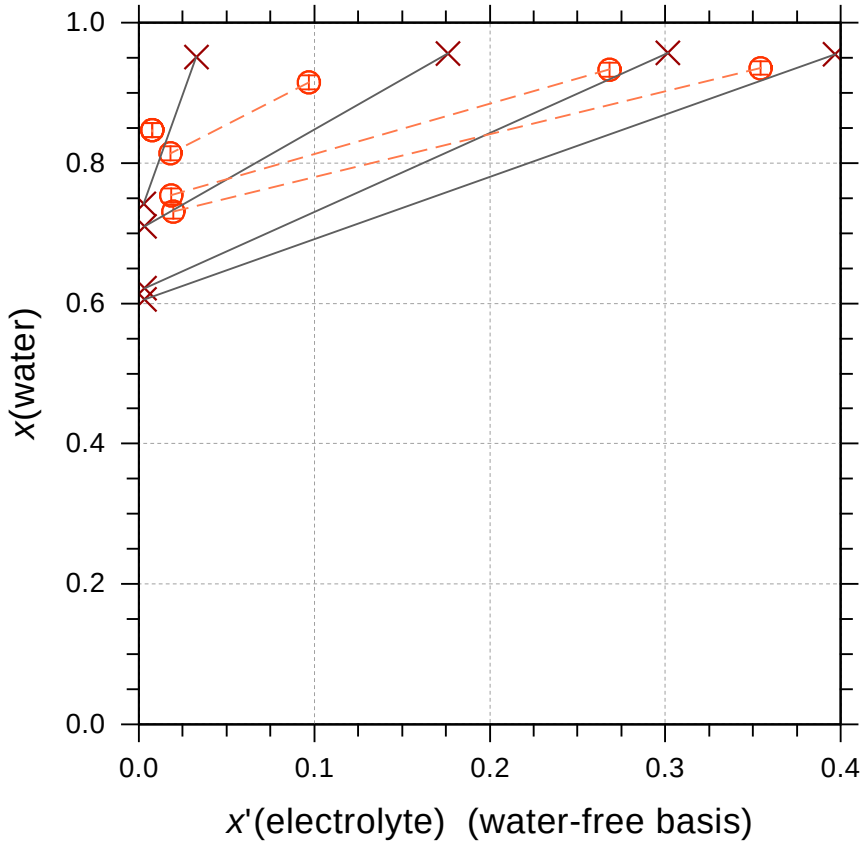


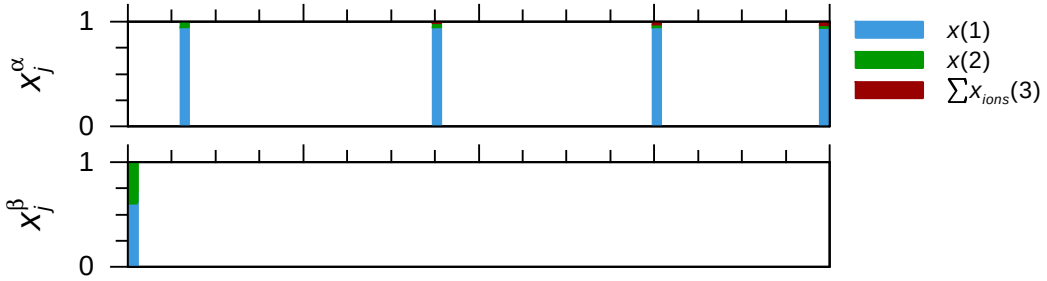
initial weighting of dataset:
$w^{init}(0941)$ = 0.010
dataset contribution to F_{obj}:
fval(0941) = 7.2480E-03
rel. contribution = 0.0034 %

Fig. S0235 (AIOMFAC_output_0356)

H_2O (1) + 2-Methylpropanoic_acid (2) + LiCl (3)

Temperature: 303 K





left y-axis:

× LiCl+2-MethylpropanoicAcid+Water_LLE_Sergeeva

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0356) = 1.000

dataset contribution to F_{obj}:

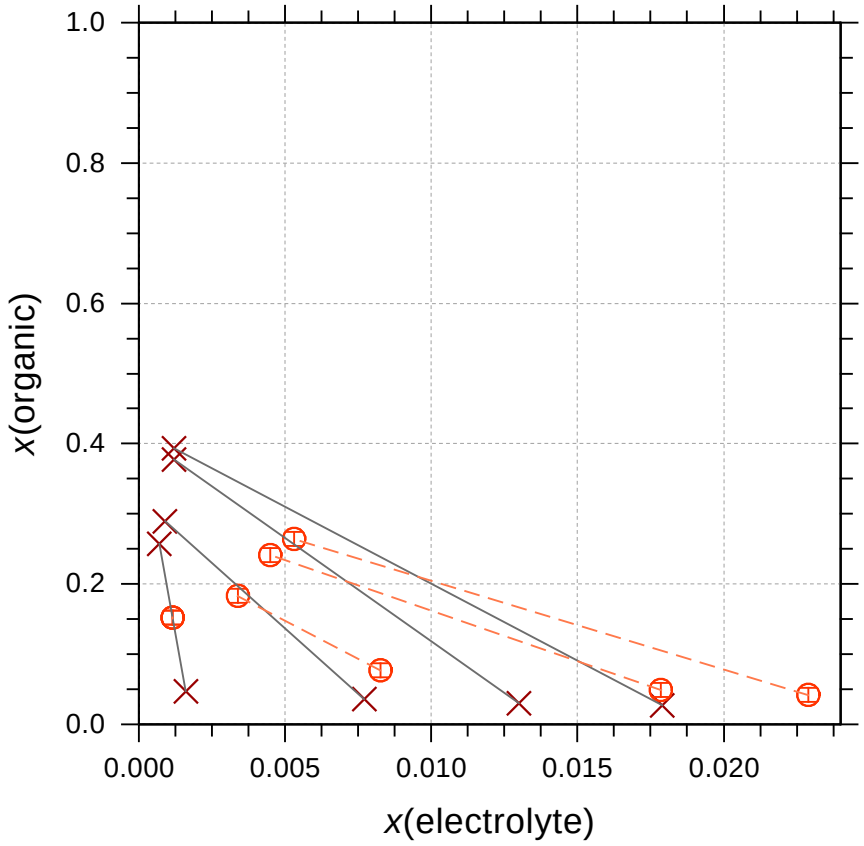
fval(0356) = 2.2305E-01

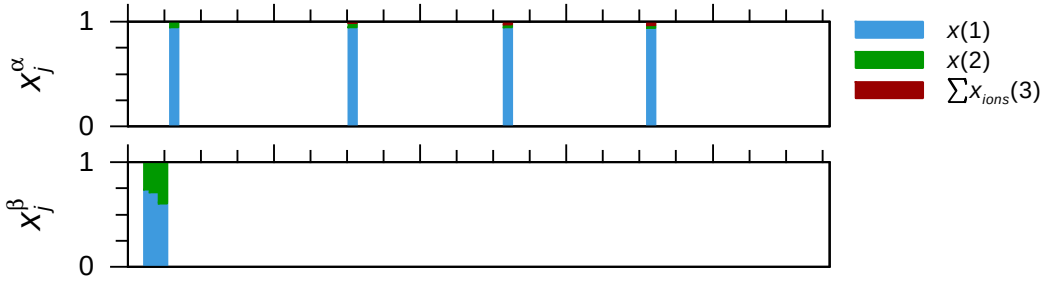
rel. contribution = 0.1061 %

Fig. S0235a (AIOMFAC_output_0356)

H_2O (1) + 2-Methylpropanoic_acid (2) + LiCl (3)

Temperature: 303 K





left y-axis:

× LiCl+2-MethylpropanoicAcid+Water_LLE_Sergeeva

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0356) = 1.000

dataset contribution to F_{obj}:

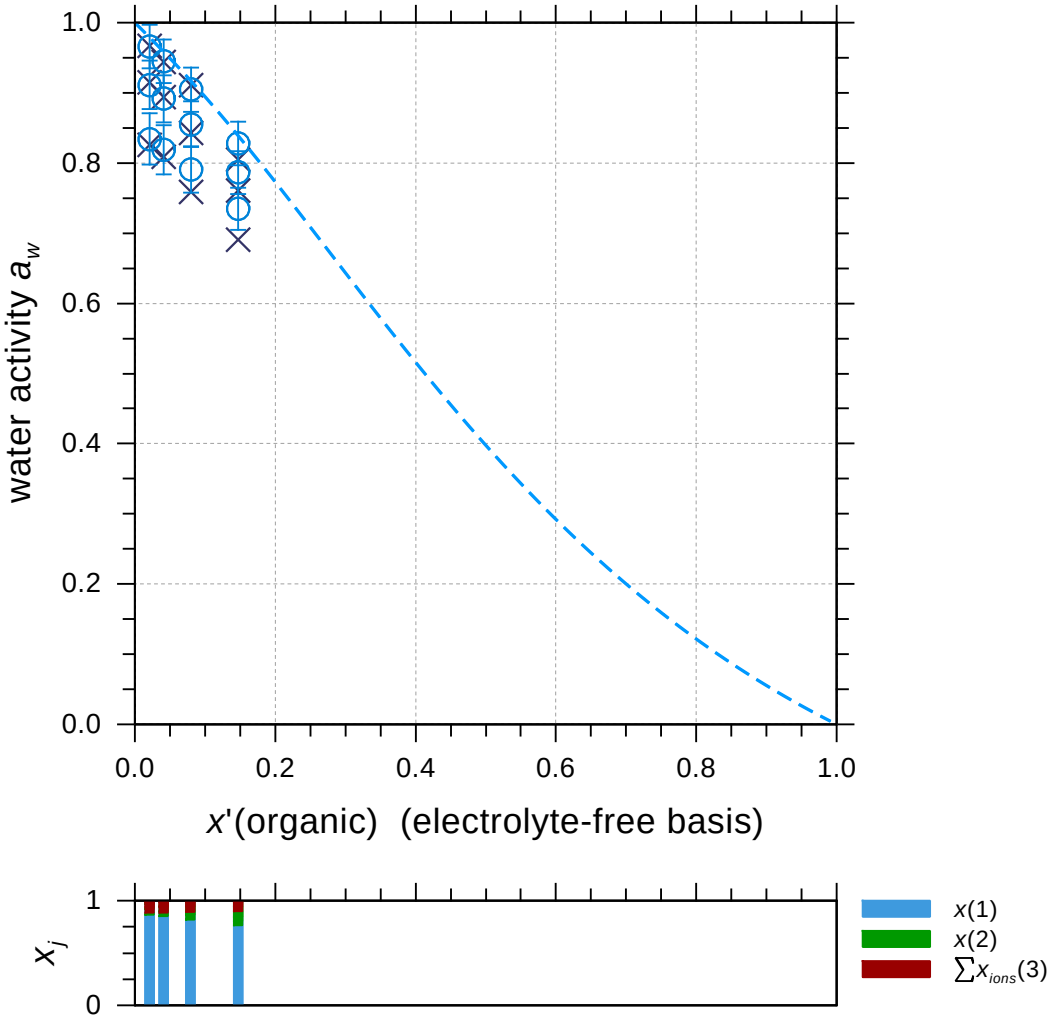
fval(0356) = 2.2305E-01

rel. contribution = 0.1061 %

Fig. S0236 (AIOMFAC_output_0388)

H_2O (1) + Malonic_acid (2) + $LiNO_3$ (3)

Temperature: 303 K

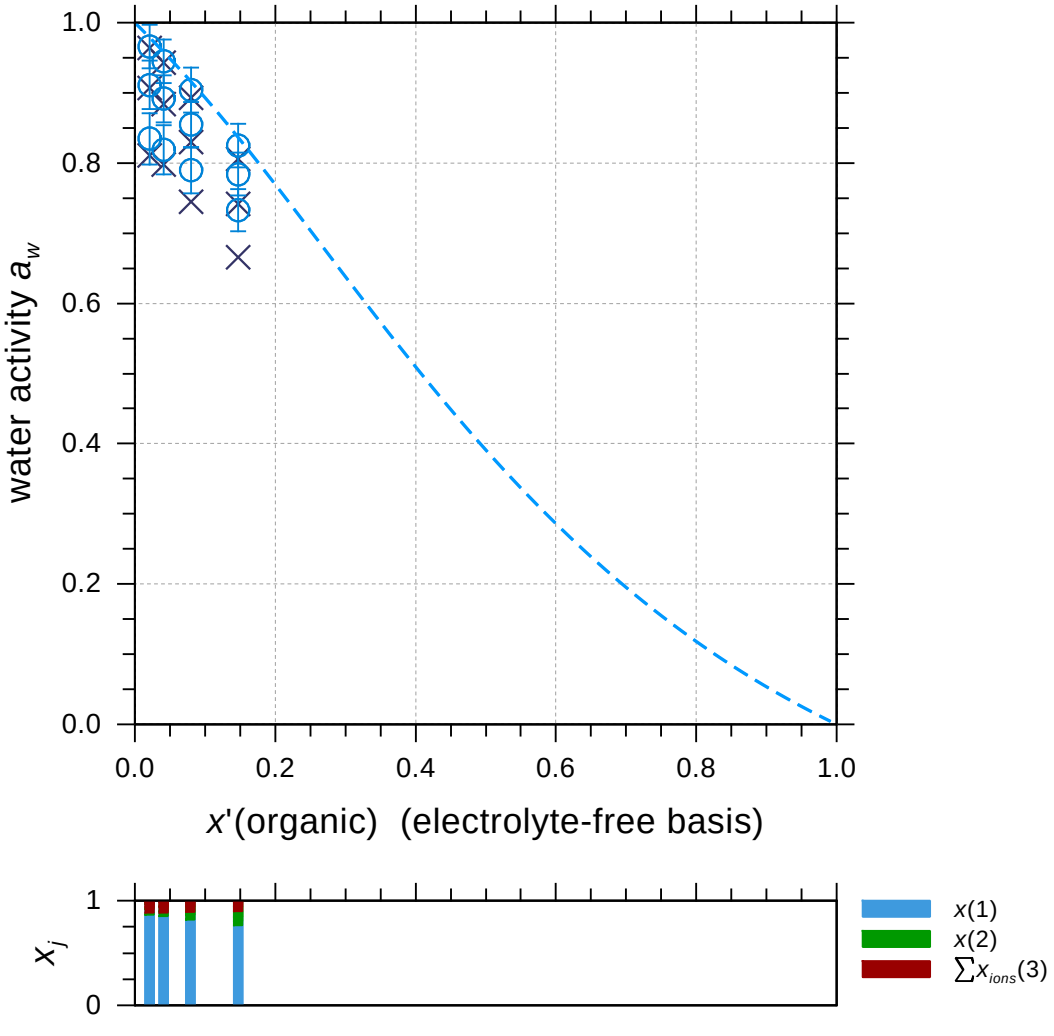


initial weighting of dataset:
$w^{init}(0388)$ = 2.000
dataset contribution to F_{obj}:
fval(0388) = 1.2616E-02
rel. contribution = 0.0060 %

Fig. S0237 (AIOMFAC_output_0389)

H_2O (1) + Malonic_acid (2) + $LiNO_3$ (3)

Temperature: 293 K

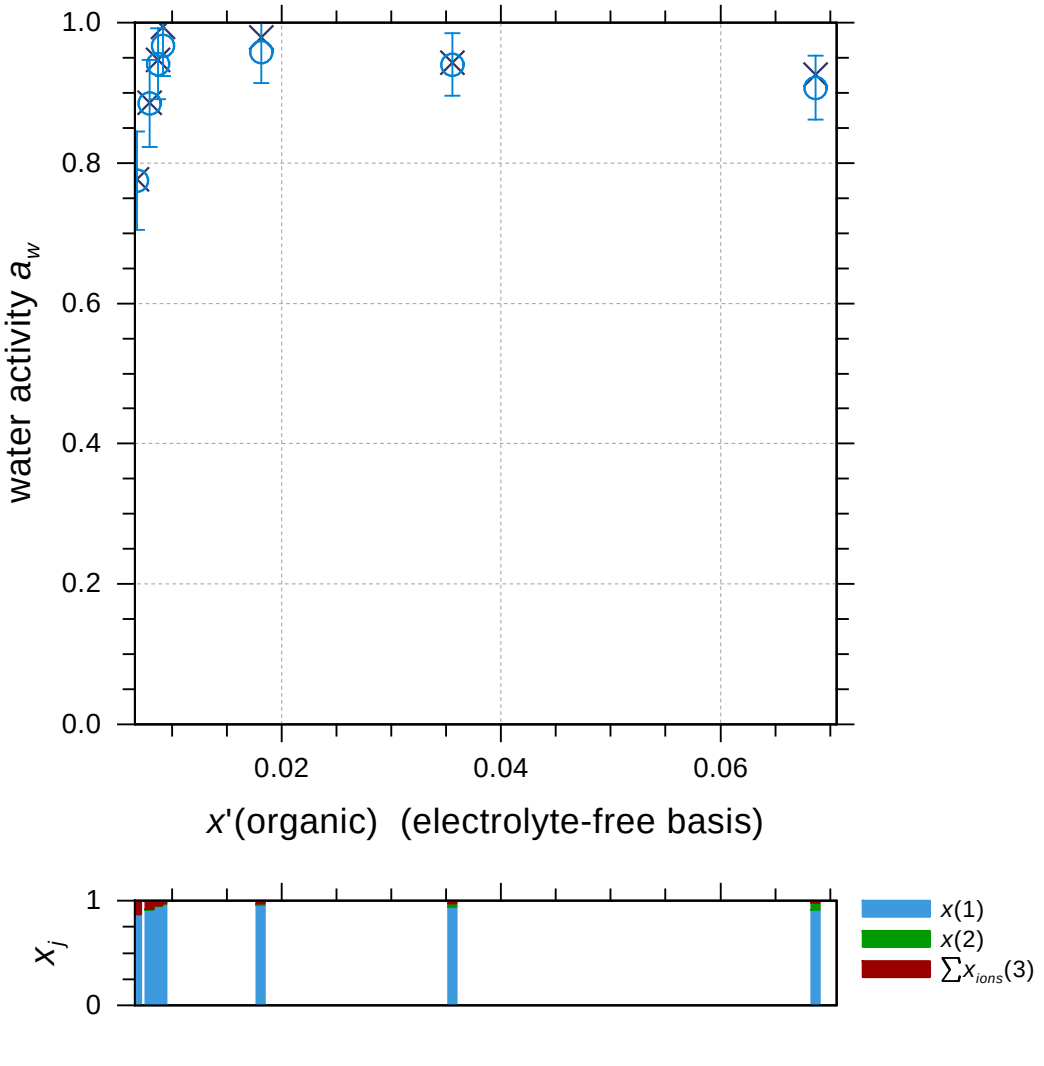


initial weighting of dataset:
$w^{init}(0389)$ = 2.000
dataset contribution to F_{obj}:
fval(0389) = 3.0942E-02
rel. contribution = 0.0147 %

Fig. S0238 (AIOMFAC_output_0969)

H_2O (1) + Maleic_acid (2) + $Mg(NO_3)_2$ (3)

Temperature: 293 K

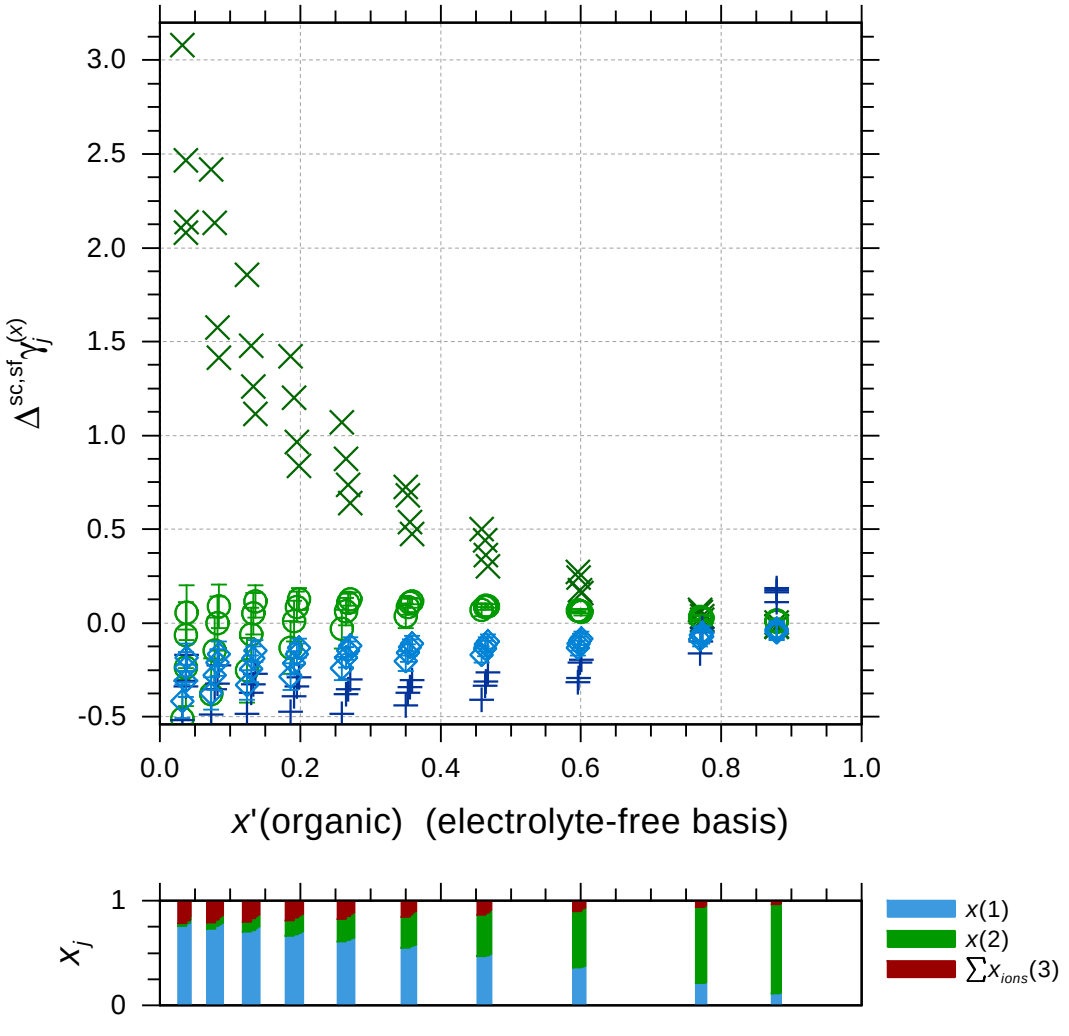


initial weighting of dataset:
$w^{init}(0969)$ = 2.000
dataset contribution to F_{obj}:
fval(0969) = 3.0556E-03
rel. contribution = 0.0015 %

Fig. S0239 (AIOMFAC_output_0946)

H_2O (1) + Formic_acid (2) + $MgCl_2$ (3)

Temperature range: 377 -- 400 K



initial weighting of dataset:

w^{init}(0946) = 0.500

dataset contribution to F_{obj}:

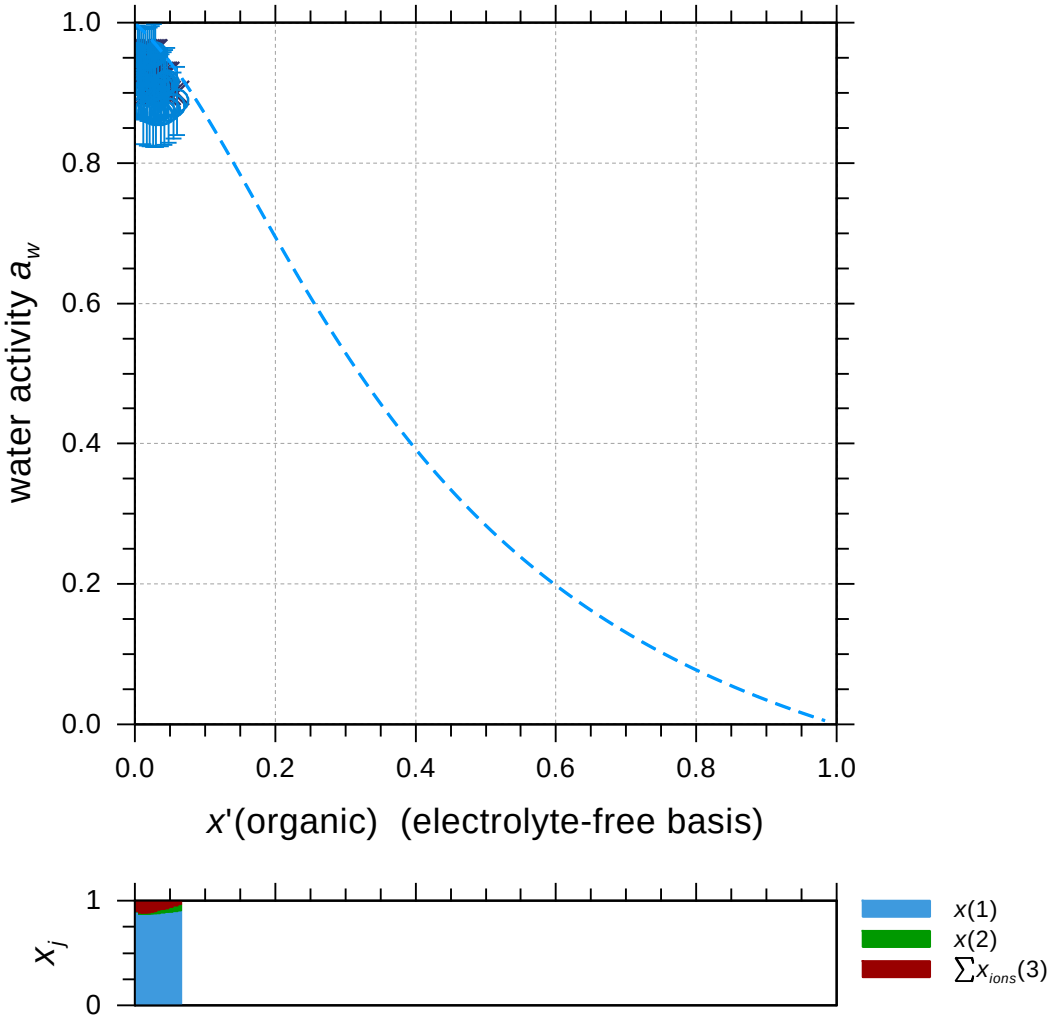
fval(0946) = 9.8660E-01

rel. contribution = 0.4692 %

Fig. S0240 (AIOMFAC_output_0302)

H_2O (1) + Citric_acid (2) + Na_2SO_4 (3)

Temperature: 298 K

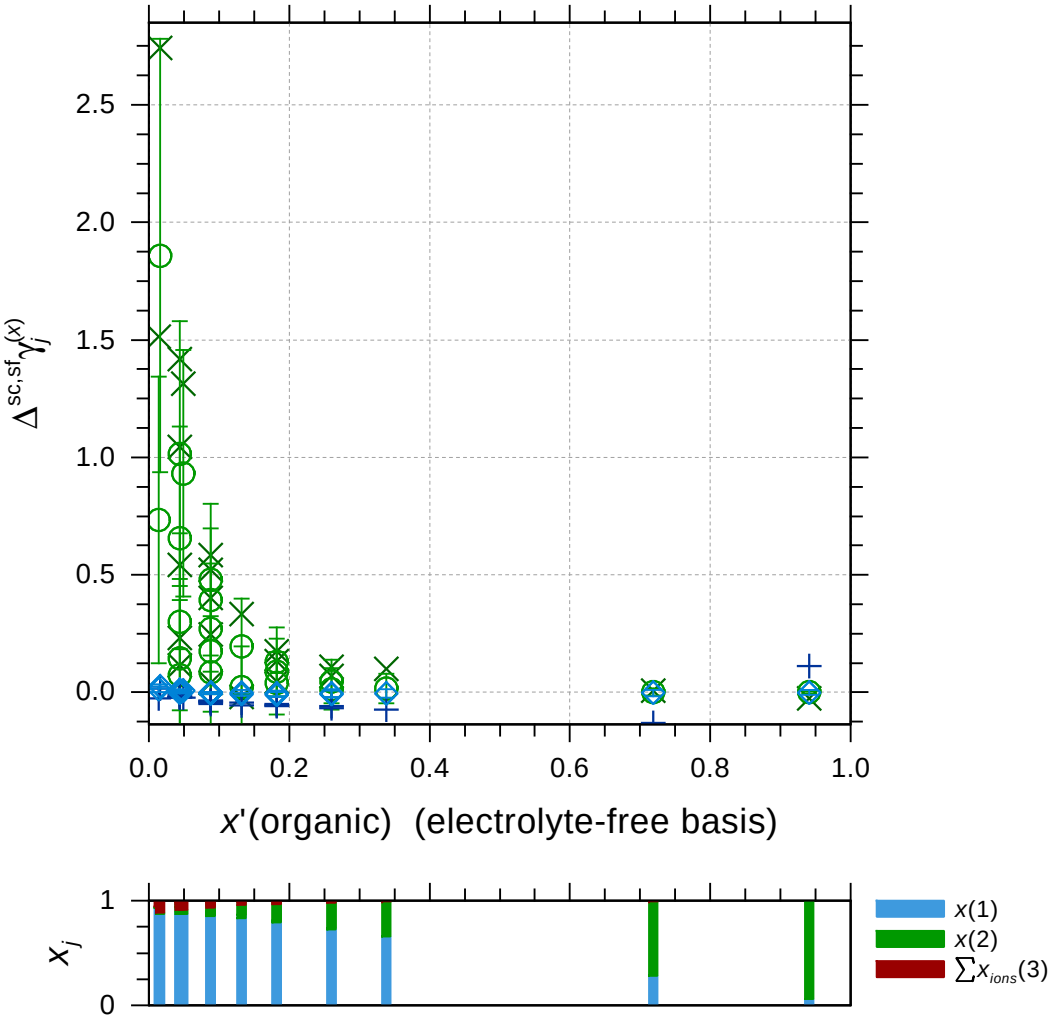


initial weighting of dataset:
w^{init}(0302) = 2.000
dataset contribution to F_{obj}:
fval(0302) = 7.1115E-03
rel. contribution = 0.0034 %

Fig. S0241 (AIOMFAC_output_0328)

H_2O (1) + Acetic_acid (2) + Na_2SO_4 (3)

Temperature range: 373 -- 388 K



initial weighting of dataset:

w^{init}(0328) = 0.500

dataset contribution to F_{obj}:

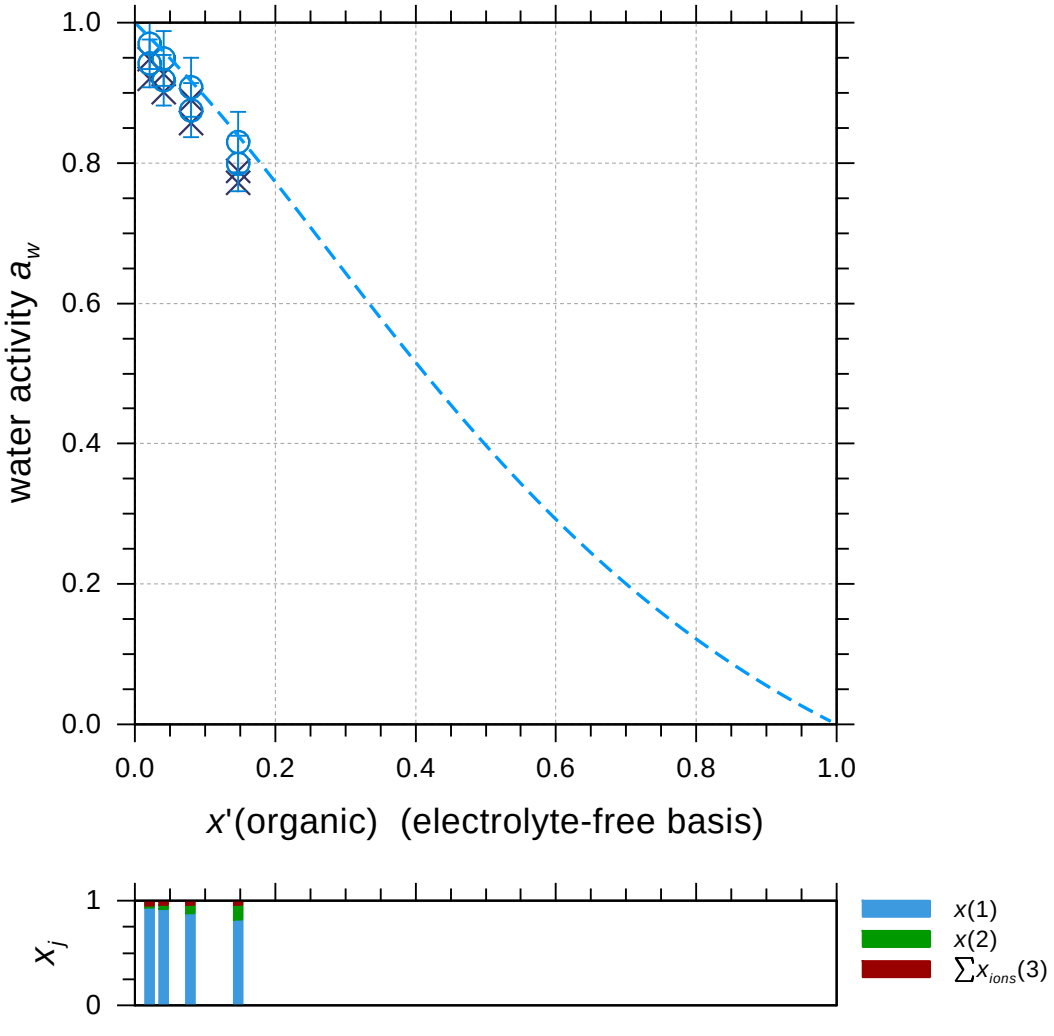
fval(0328) = 5.8791E-02

rel. contribution = 0.0280 %

Fig. S0242 (AIOMFAC_output_0384)

H_2O (1) + Malonic_acid (2) + Na_2SO_4 (3)

Temperature: 303 K

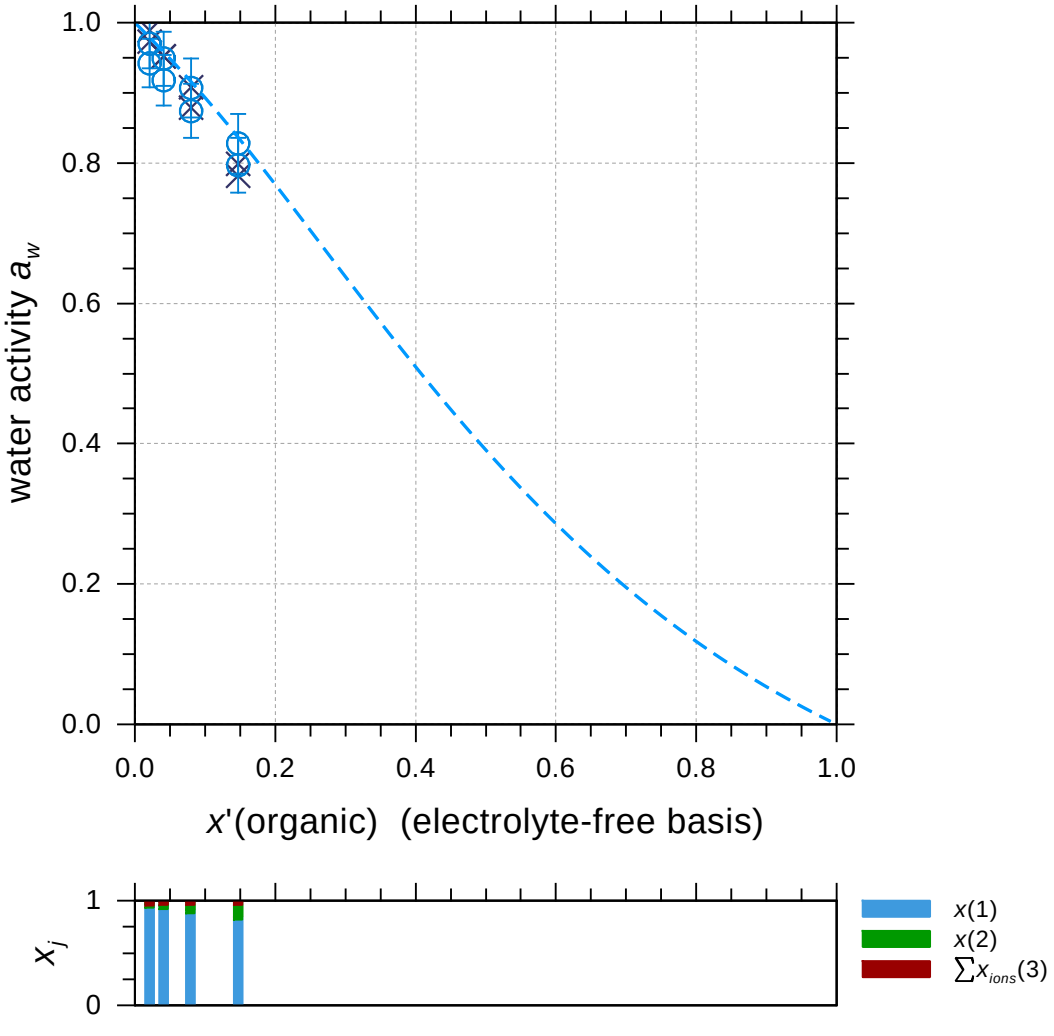


initial weighting of dataset:
$w^{init}(0384)$ = 2.000
dataset contribution to F_{obj}:
fval(0384) = 2.1096E-02
rel. contribution = 0.0100 %

Fig. S0243 (AIOMFAC_output_0385)

H_2O (1) + Malonic_acid (2) + Na_2SO_4 (3)

Temperature: 293 K

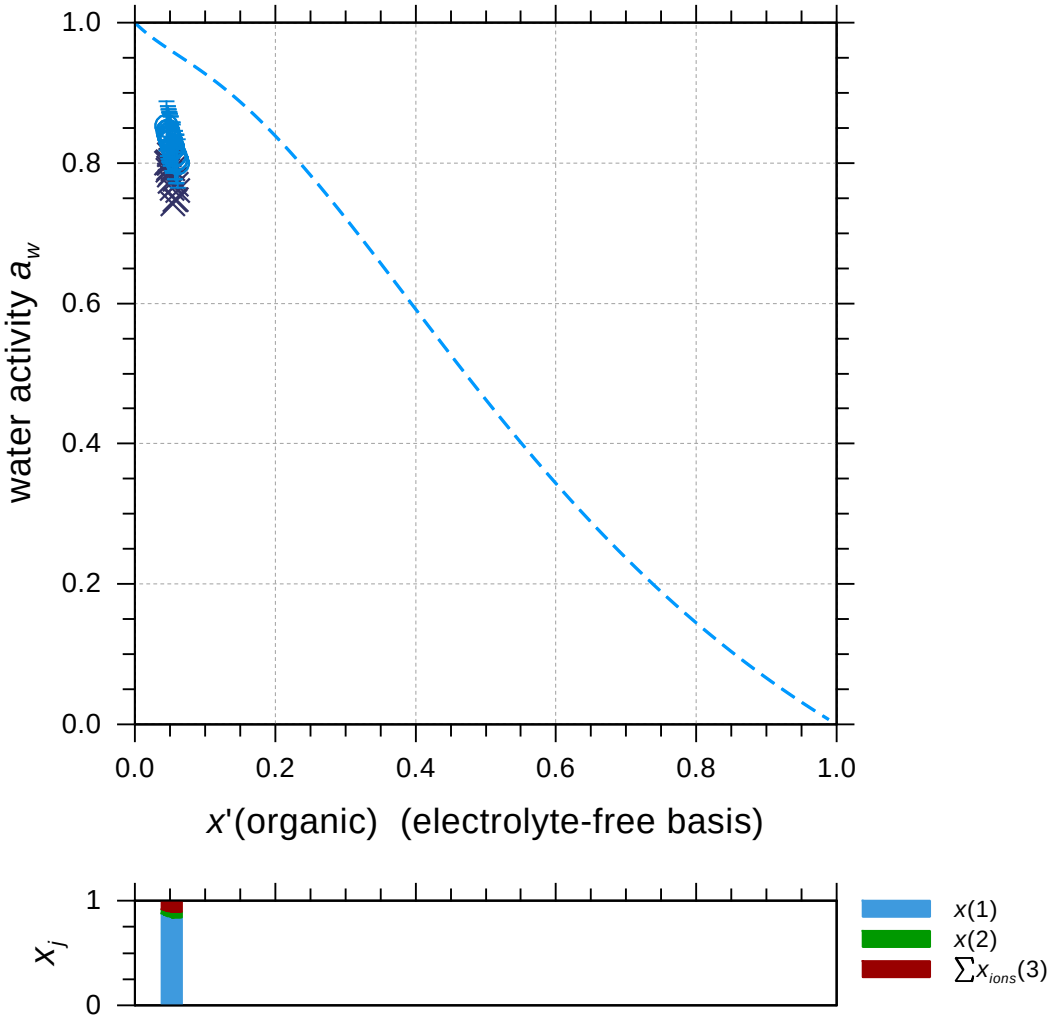


initial weighting of dataset:
$w^{init}(0385)$ = 2.000
dataset contribution to F_{obj}:
fval(0385) = 7.8950E-03
rel. contribution = 0.0038 %

Fig. S0244 (AIOMFAC_output_0262)

H_2O (1) + Glutaric_acid (2) + NaCl (3)

Temperature: 295 K

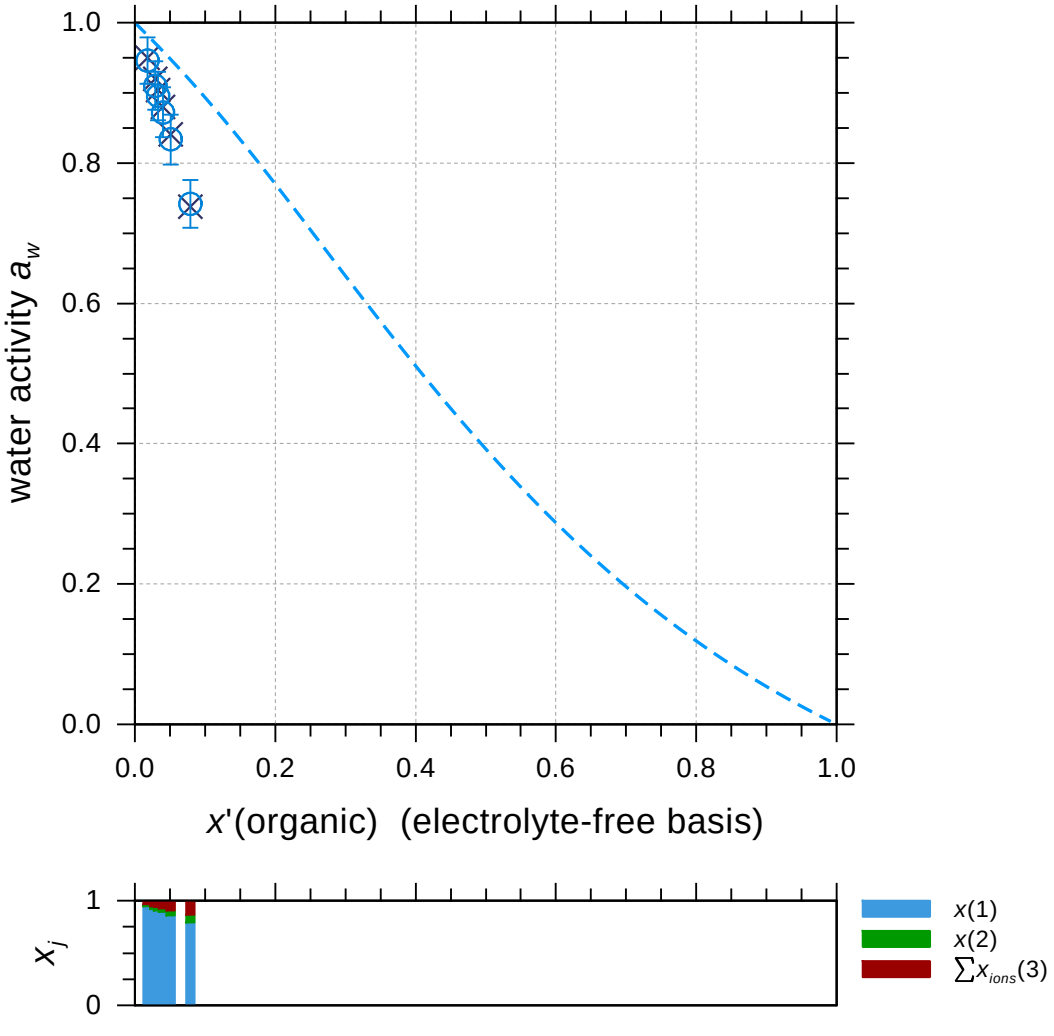


initial weighting of dataset:
$w^{init}(0262)$ = 1.000
dataset contribution to F_{obj}:
fval(0262) = 3.6471E-02
rel. contribution = 0.0173 %

Fig. S0245 (AIOMFAC_output_0263)

H_2O (1) + Malonic_acid (2) + NaCl (3)

Temperature: 295 K

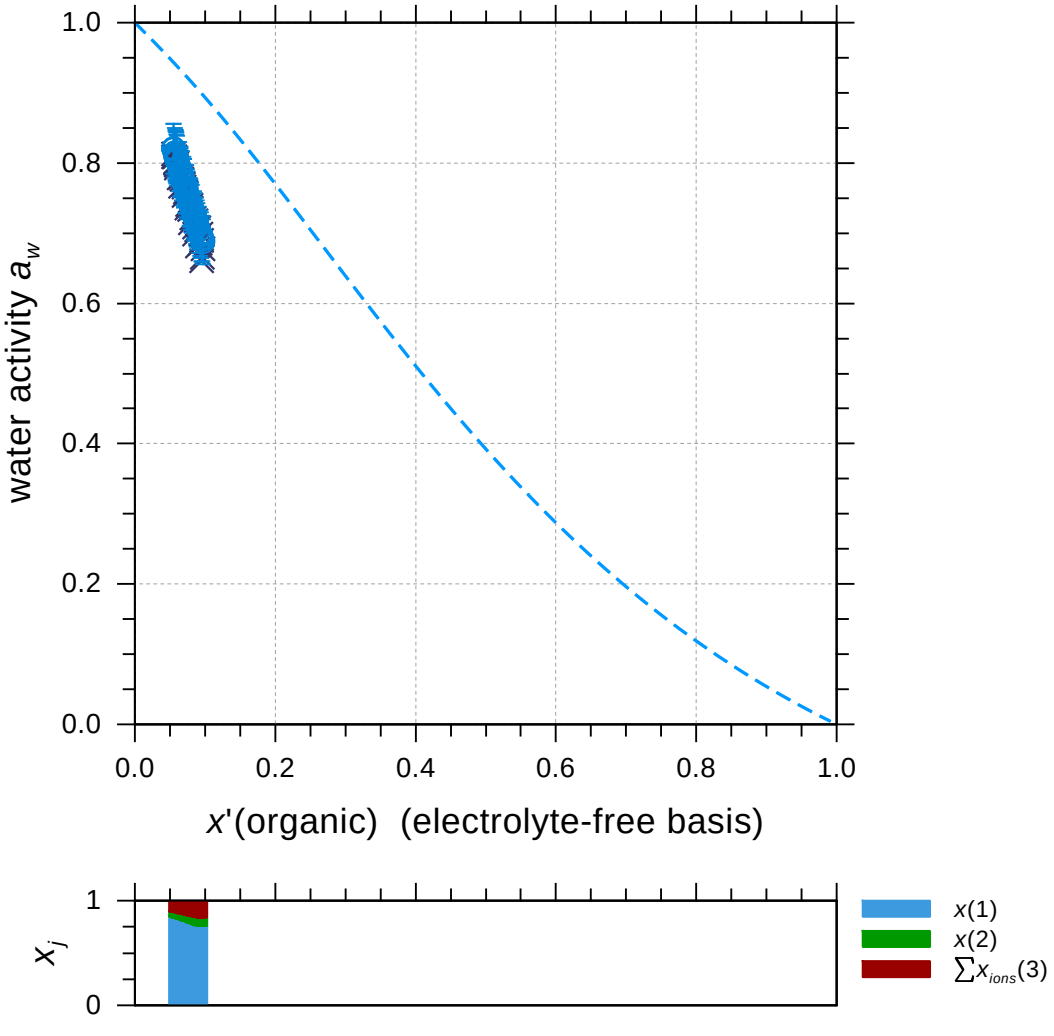


initial weighting of dataset:
$w^{init}(0263)$ = 2.000
dataset contribution to F_{obj}:
fval(0263) = 7.4440E-04
rel. contribution = 0.0004 %

Fig. S0246 (AIOMFAC_output_0264)

H_2O (1) + Malonic_acid (2) + NaCl (3)

Temperature: 295 K

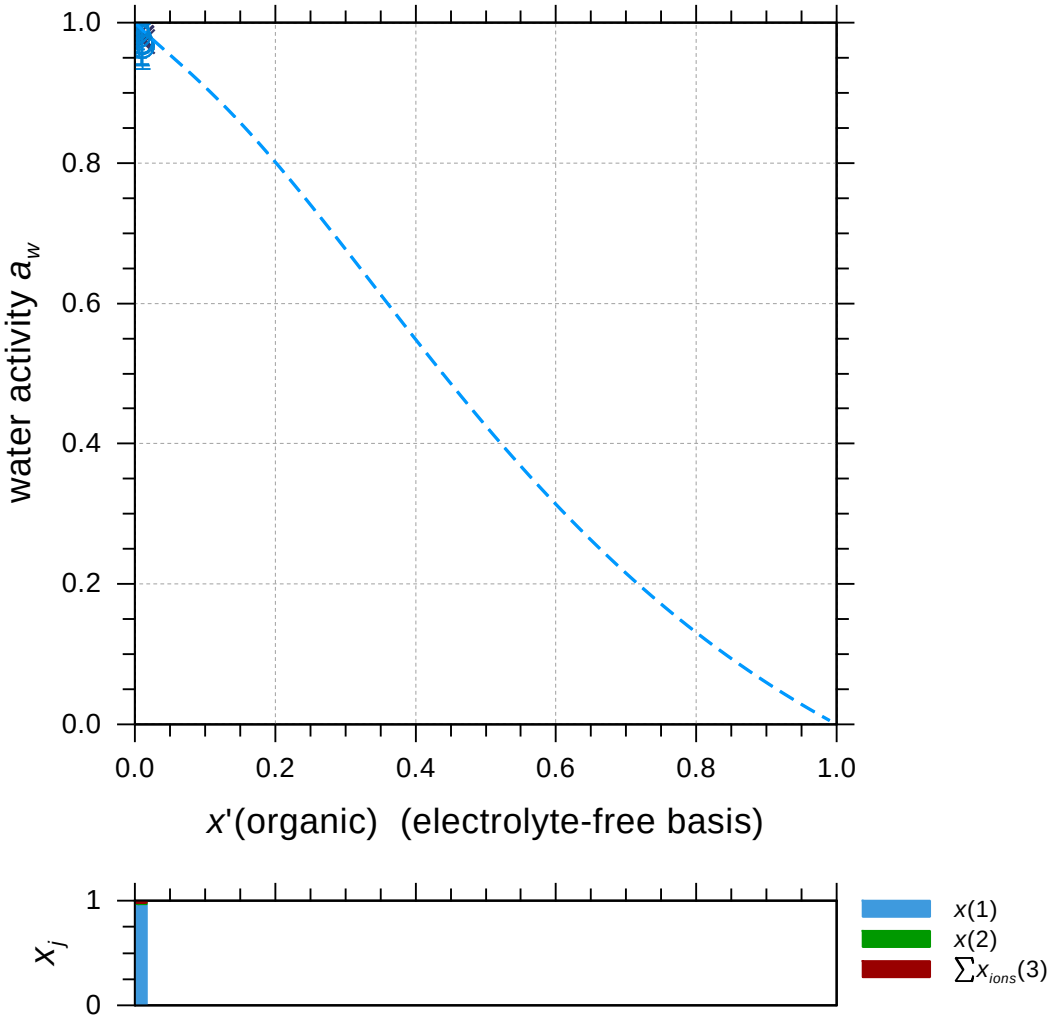


initial weighting of dataset:
$w^{init}(0264)$ = 1.000
dataset contribution to F_{obj}:
fval(0264) = 3.4148E-03
rel. contribution = 0.0016 %

Fig. S0247 (AIOMFAC_output_0265)

H_2O (1) + Succinic_acid (2) + NaCl (3)

Temperature: 295 K

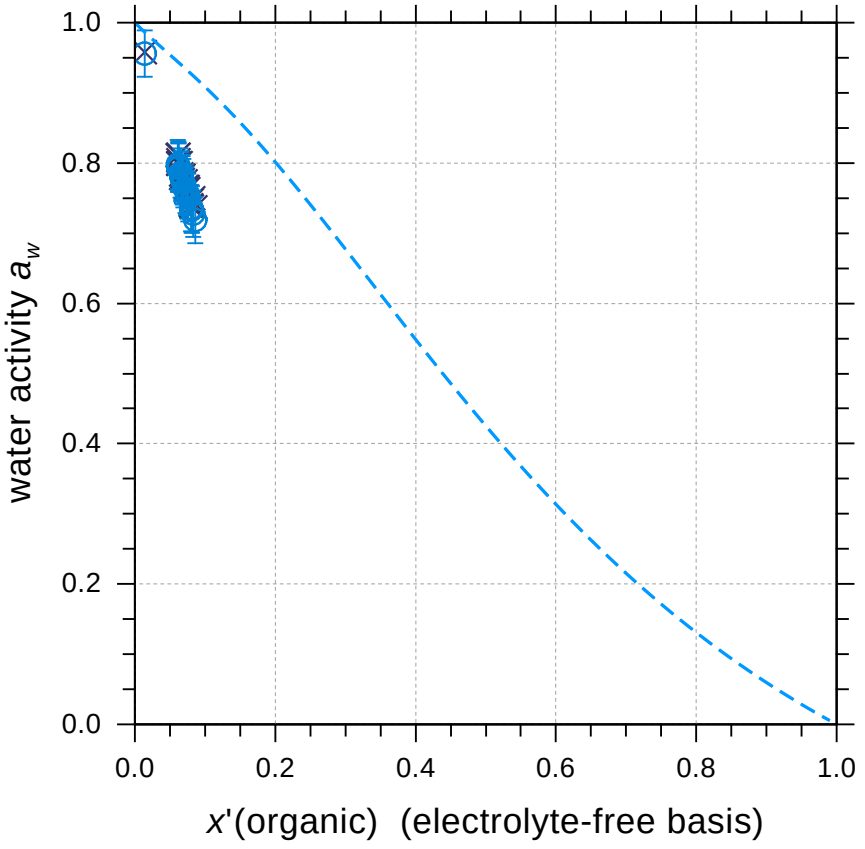


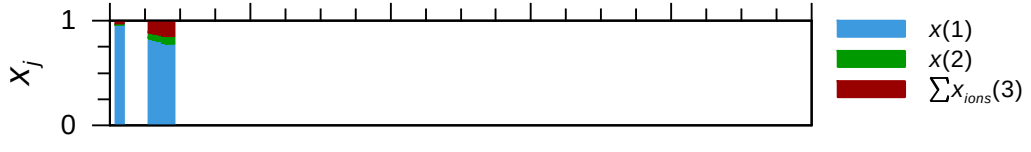
initial weighting of dataset:
w^{init}(0265) = 2.000
dataset contribution to F_{obj}:
fval(0265) = 3.4625E-04
rel. contribution = 0.0002 %

Fig. S0248 (AIOMFAC_output_0266)

H_2O (1) + Succinic_acid (2) + NaCl (3)

Temperature: 295 K



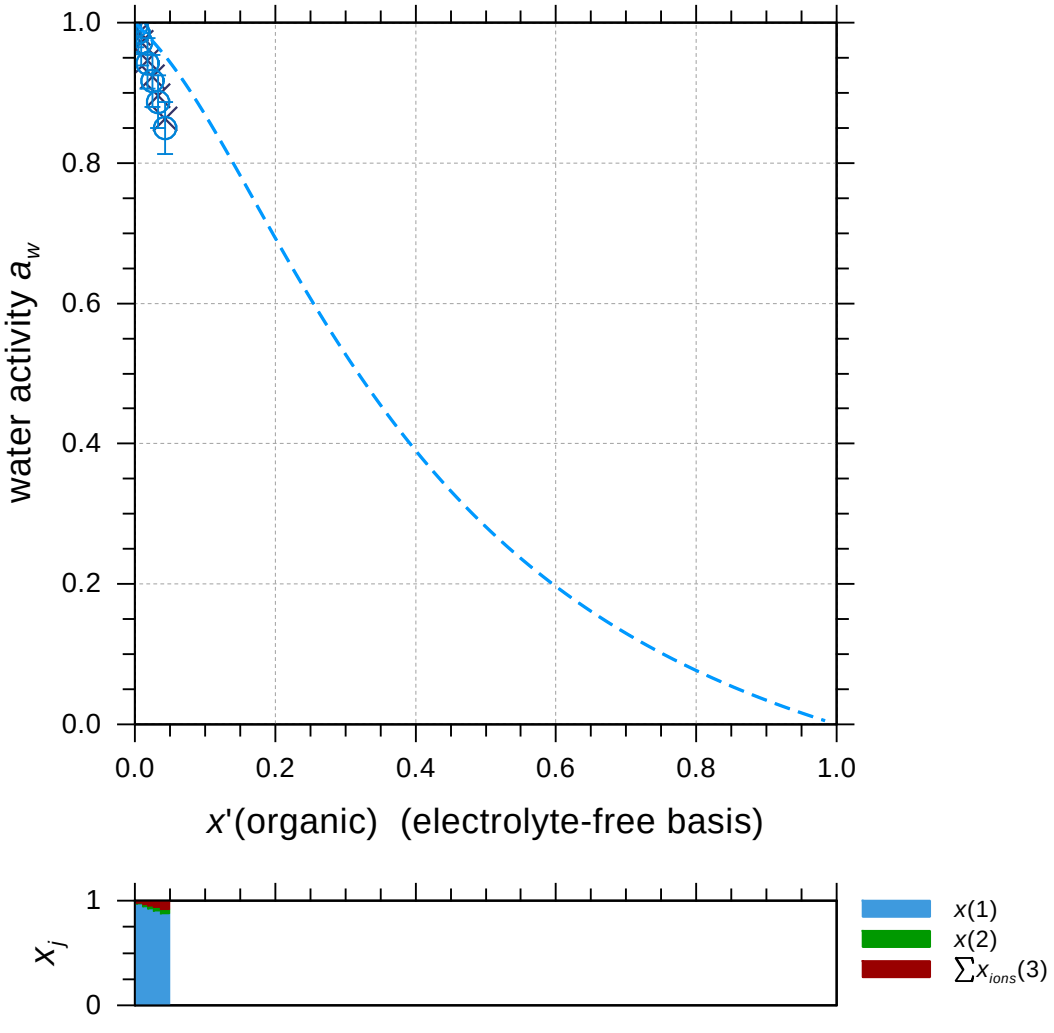


initial weighting of dataset:
$w^{init}(0266)$ = 1.000
dataset contribution to F_{obj}:
fval(0266) = 1.7263E-03
rel. contribution = 0.0008 %

Fig. S0249 (AIOMFAC_output_0267)

H_2O (1) + Citric_acid (2) + NaCl (3)

Temperature: 295 K

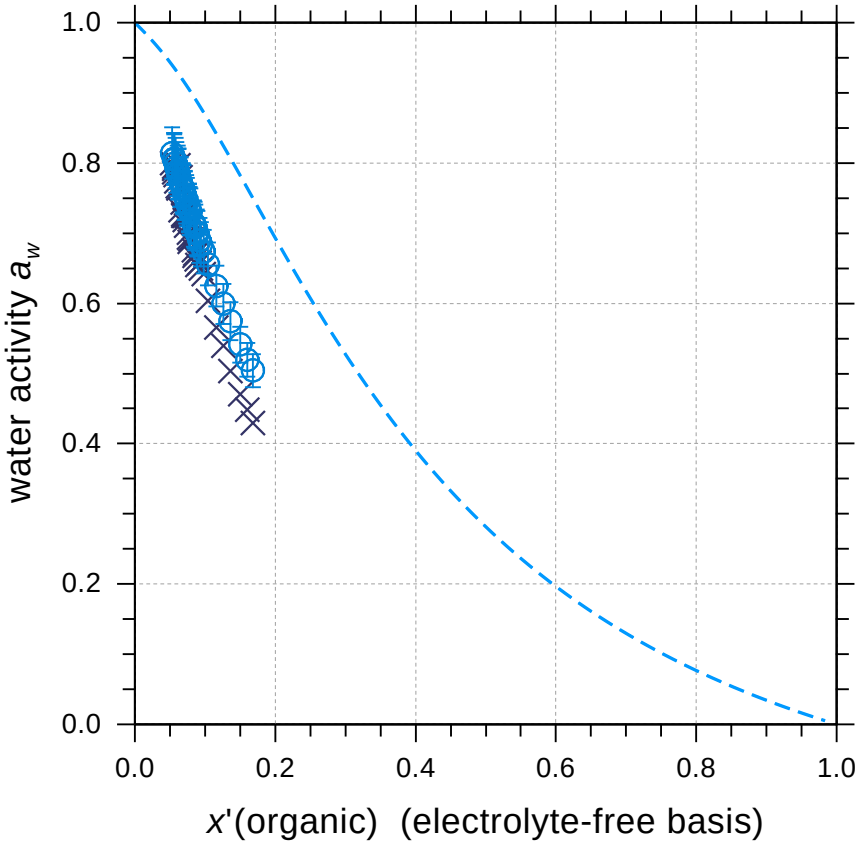


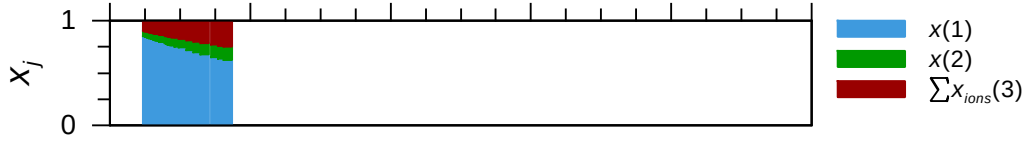
initial weighting of dataset:
$w^{init}(0267)$ = 2.000
dataset contribution to F_{obj}:
fval(0267) = 7.5710E-04
rel. contribution = 0.0004 %

Fig. S0250 (AIOMFAC_output_0268)

H_2O (1) + Citric_acid (2) + NaCl (3)

Temperature: 295 K





initial weighting of dataset:
$w^{init}(0268)$ = 1.000
dataset contribution to F_{obj}:
fval(0268) = 4.6104E-02
rel. contribution = 0.0219 %

left y-axis:

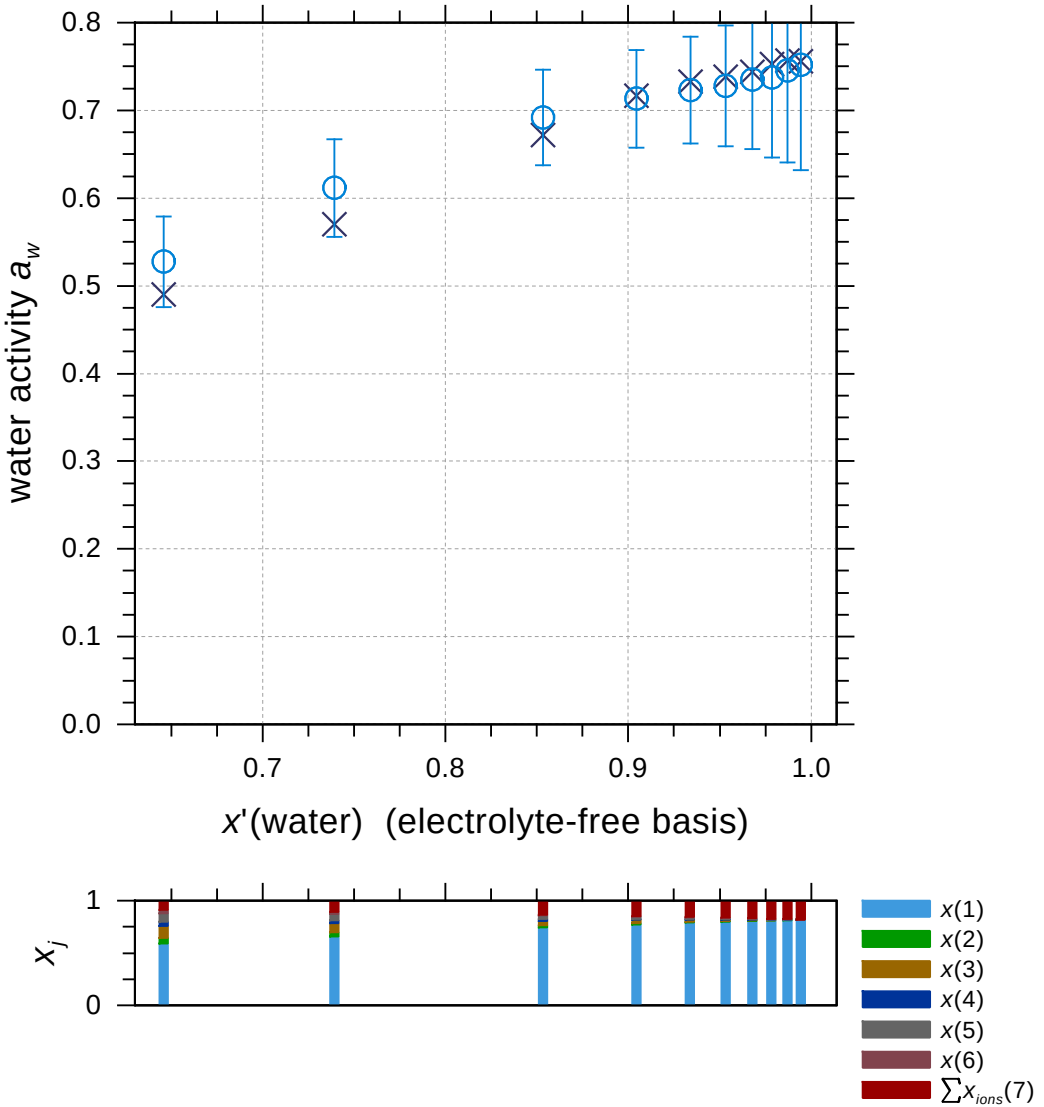
× NaCl+DicarboxylicAcidsMixtureM5+Water_aw_Marcolli

○ AIOMFAC water activity a_w

Fig. S0251 (AIOMFAC_output_0286)

H_2O (1) + Malic_acid (2) + Malonic_acid (3) + Maleic_acid (4) + Glutaric_acid (5) + Methylsuccinic_acid (6) + NaCl (7)

Temperature: 298 K



initial weighting of dataset:
$w^{init}(0286)$ = 2.000
dataset contribution to F_{obj}:
fval(0286) = 2.1895E-02
rel. contribution = 0.0104 %

left y-axis:

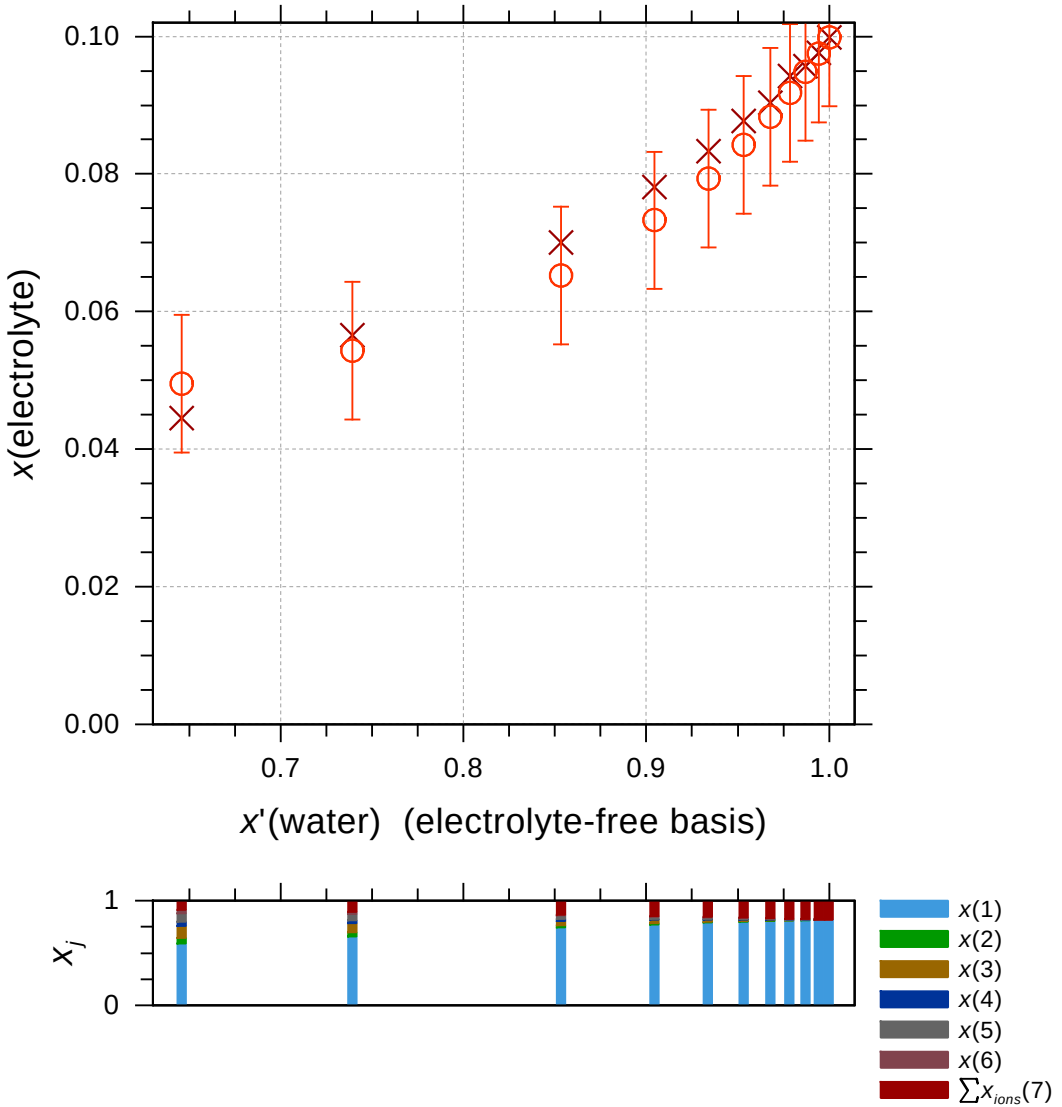
× NaCl+DicarboxylicAcidsMixtureM5+Water_SLE-salt_Marcolli

○ AIOMFAC calc. SLE composition

Fig. S0252 (AIOMFAC_output_0287)

H_2O (1) + Malic_acid (2) + Malonic_acid (3) + Maleic_acid (4) + Glutaric_acid (5) + Methylsuccinic_acid (6) + NaCl (7)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0287)$ = 1.000

dataset contribution to F_{obj}:

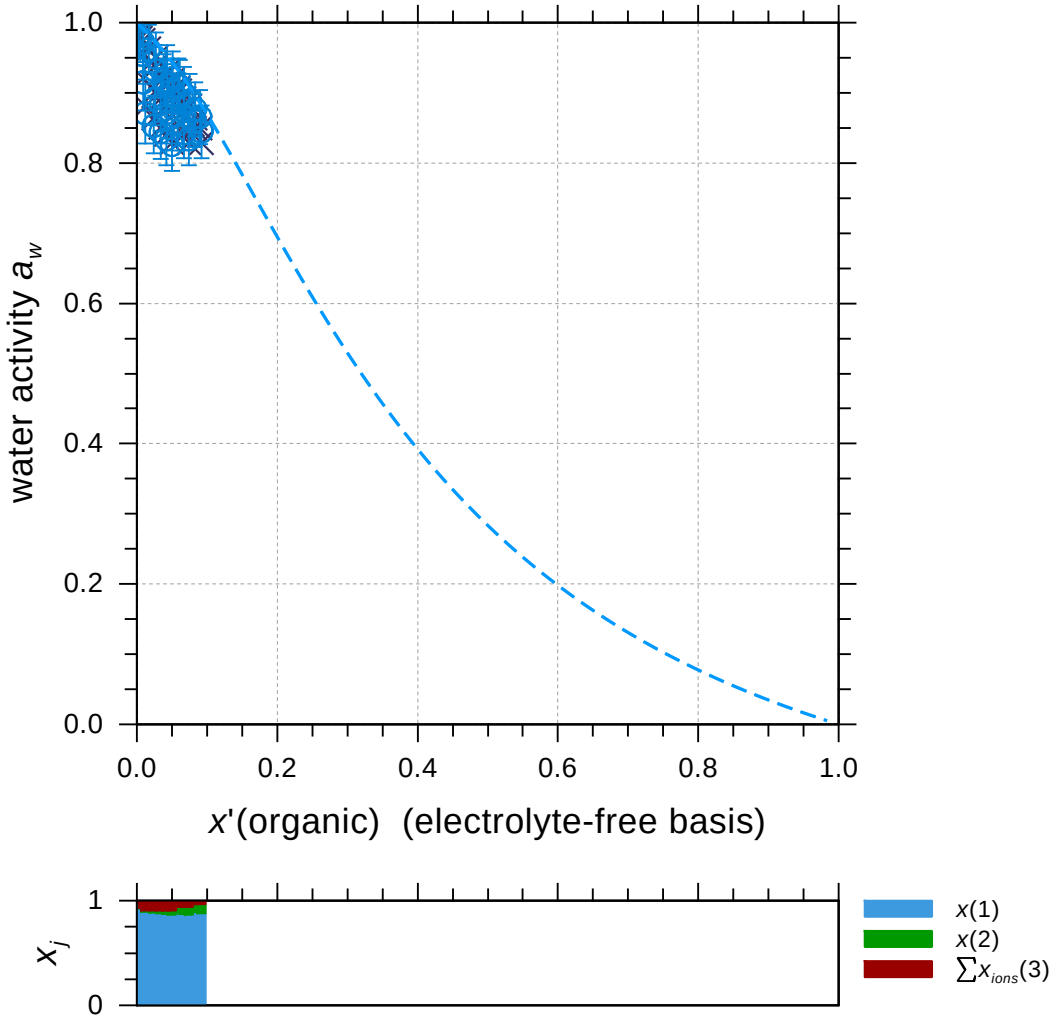
fval(0287) = 1.9214E-02

rel. contribution = 0.0091 %

Fig. S0253 (AIOMFAC_output_0300)

H_2O (1) + Citric_acid (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:
$w^{init}(0300)$ = 2.000
dataset contribution to F_{obj}:
fval(0300) = 1.0974E-03
rel. contribution = 0.0005 %

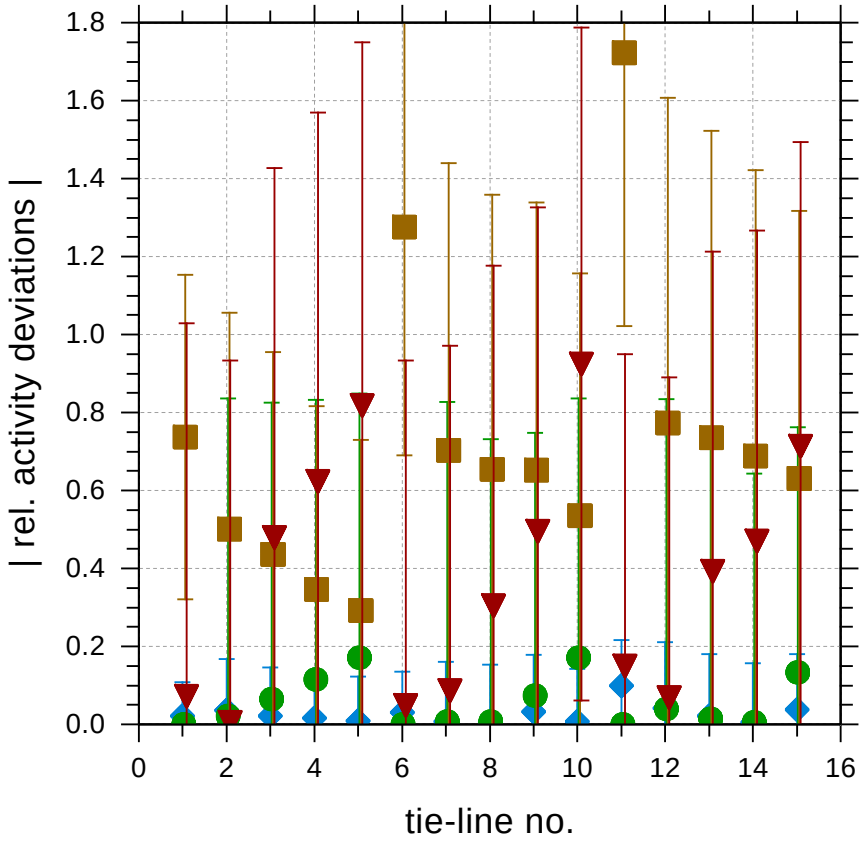
Fig. S0254 (AIOMFAC_output_0310)

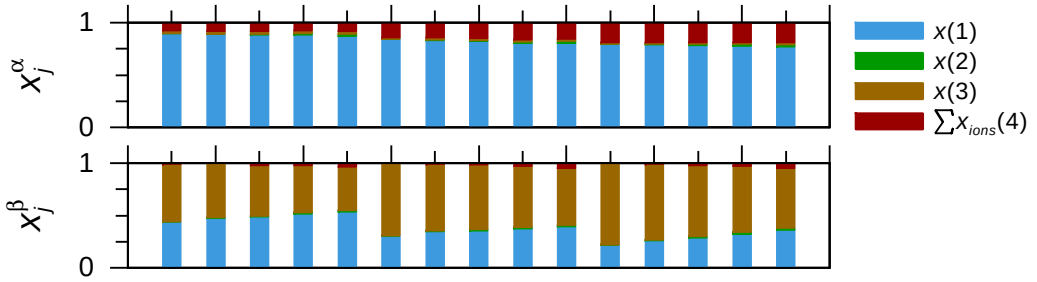
H_2O (1) + Citric_acid (2) + 2-Butanol (3) + NaCl (4)

Temperature: 298 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)





initial weighting of dataset:
$w^{init}(0310)$ = 1.000
dataset contribution to F_{obj}:
fval(0310) = 4.3192E+00
rel. contribution = 2.0539 %

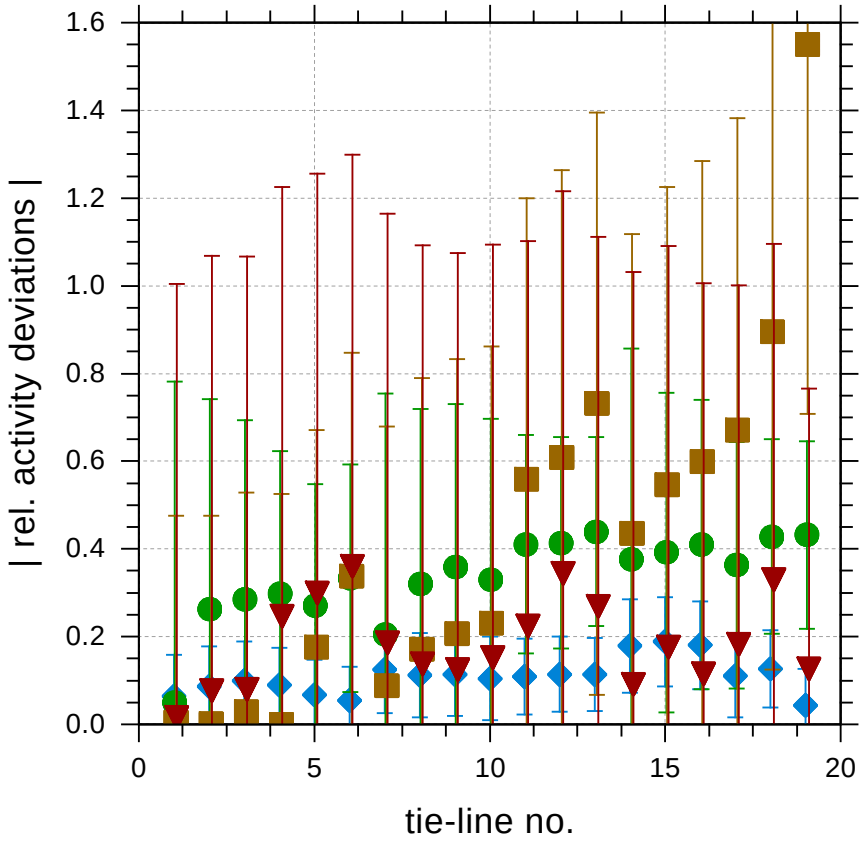
Fig. S0255 (AIOMFAC_output_0312)

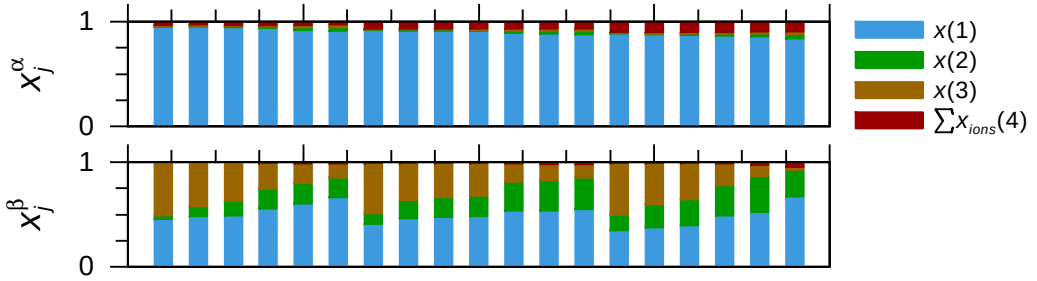
H_2O (1) + Propanoic_acid (2) + 1-Butanol (3) + NaCl (4)

Temperature: 303 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



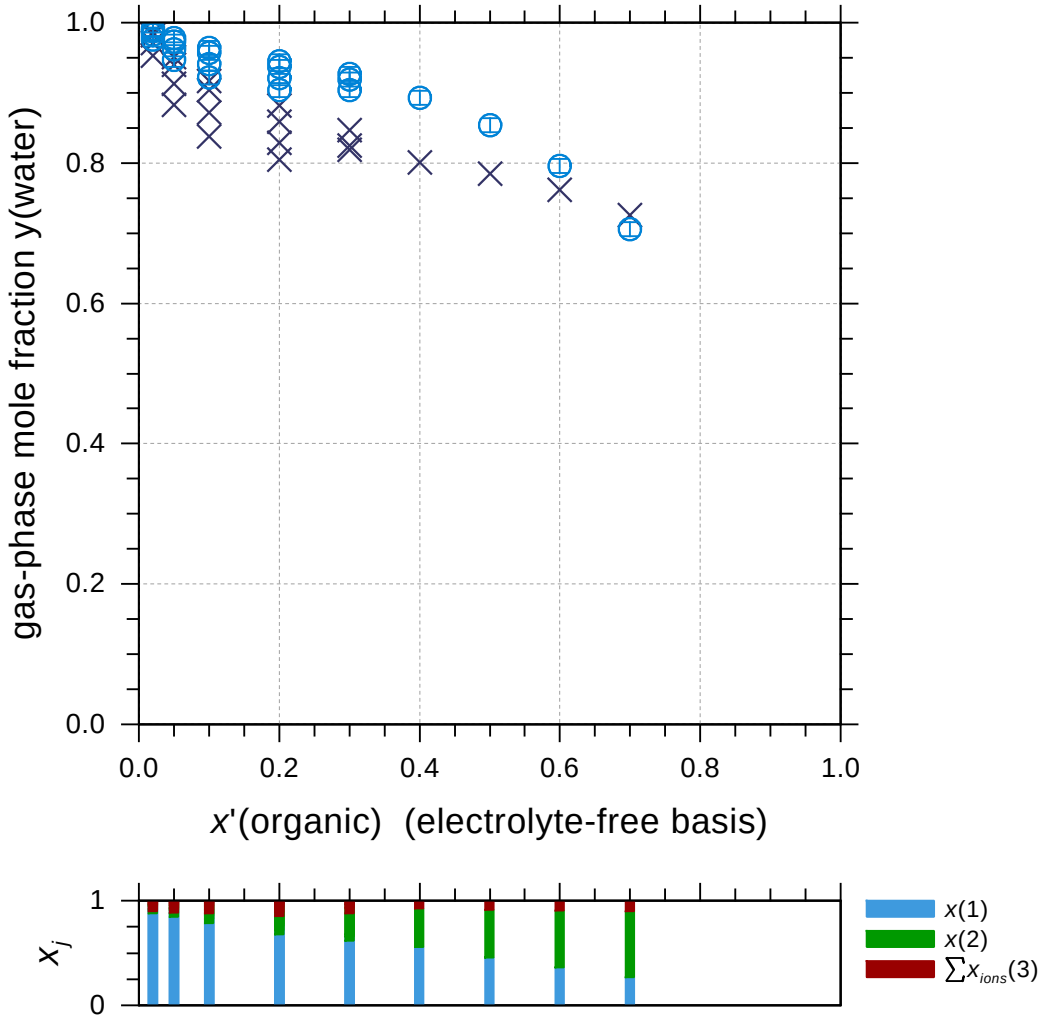


initial weighting of dataset:
$w^{init}(0312)$ = 1.000
dataset contribution to F_{obj}:
fval(0312) = 2.4732E+00
rel. contribution = 1.1761 %

Fig. S0256 (AIOMFAC_output_0331)

H_2O (1) + Propanoic_acid (2) + NaCl (3)

Temperature: 333 K

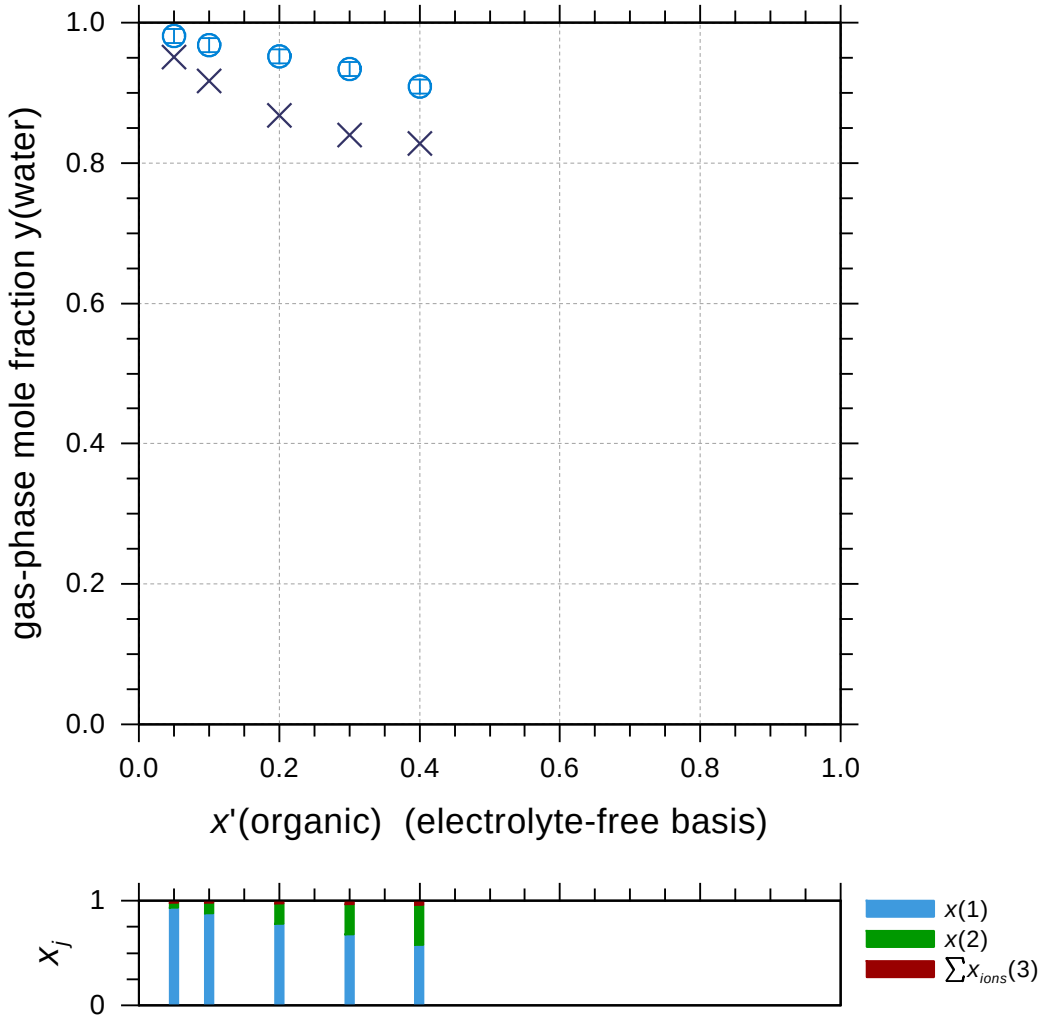


initial weighting of dataset:
$w^{init}(0331)$ = 0.500
dataset contribution to F_{obj}:
fval(0331) = 2.7601E-02
rel. contribution = 0.0131 %

Fig. S0257 (AIOMFAC_output_0338)

H_2O (1) + Propanoic_acid (2) + NaCl (3)

Temperature: 313 K

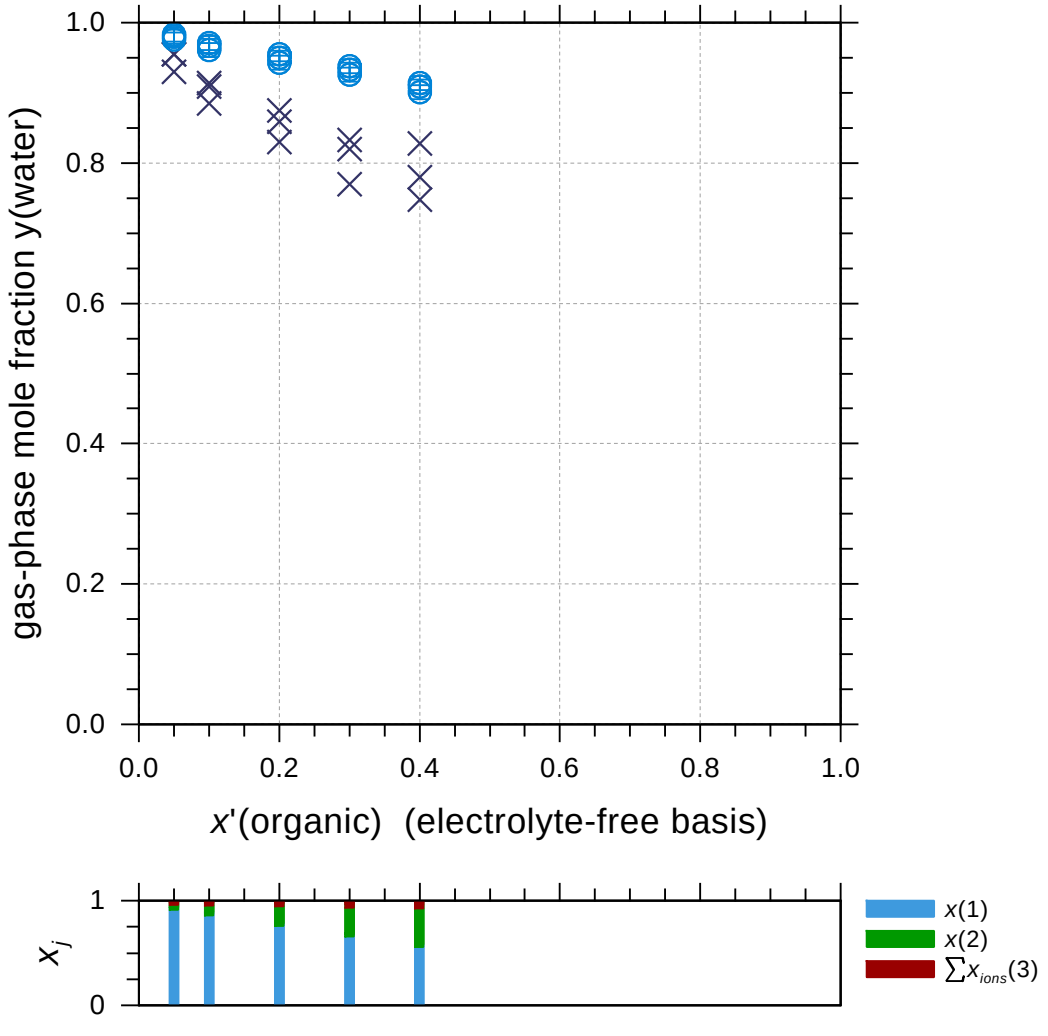


initial weighting of dataset:
$w^{init}(0338)$ = 0.500
dataset contribution to F_{obj}:
fval(0338) = 1.7377E-02
rel. contribution = 0.0083 %

Fig. S0258 (AIOMFAC_output_0339)

H_2O (1) + Propanoic_acid (2) + NaCl (3)

Temperature: 323 K

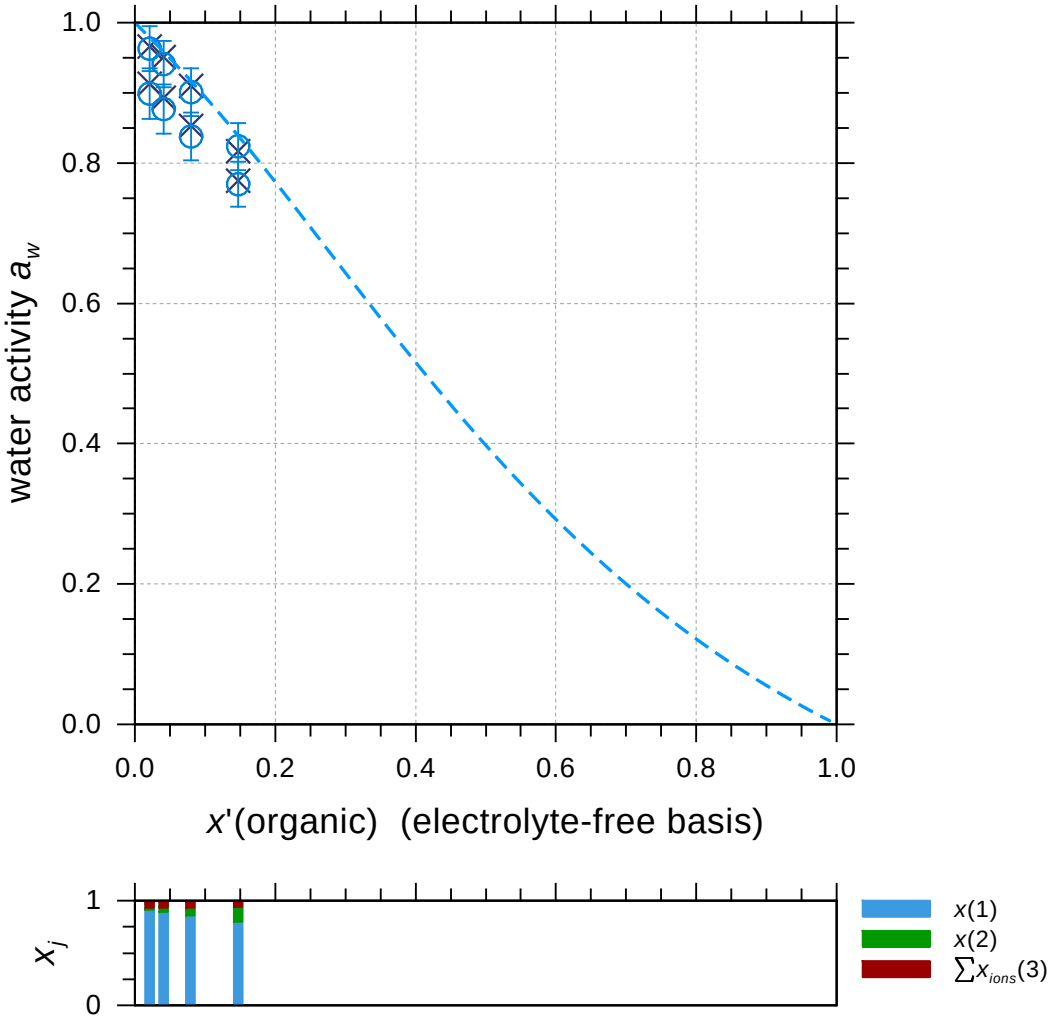


initial weighting of dataset:
$w^{init}(0339)$ = 0.500
dataset contribution to F_{obj}:
fval(0339) = 6.9116E-02
rel. contribution = 0.0329 %

Fig. S0259 (AIOMFAC_output_0386)

H_2O (1) + Malonic_acid (2) + NaCl (3)

Temperature: 303 K

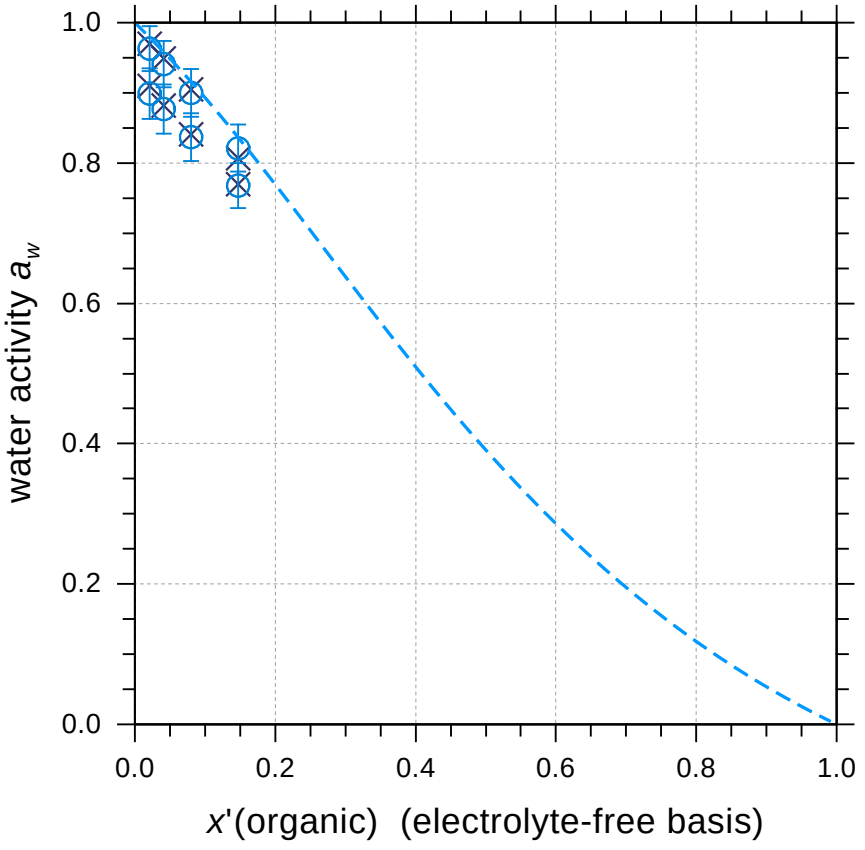


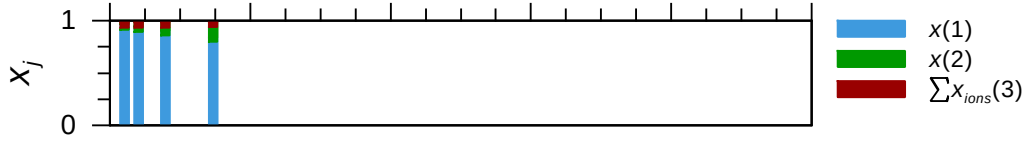
initial weighting of dataset:
$w^{init}(0386)$ = 2.000
dataset contribution to F_{obj}:
fval(0386) = 2.2899E-03
rel. contribution = 0.0011 %

Fig. S0260 (AIOMFAC_output_0387)

H_2O (1) + Malonic_acid (2) + NaCl (3)

Temperature: 293 K



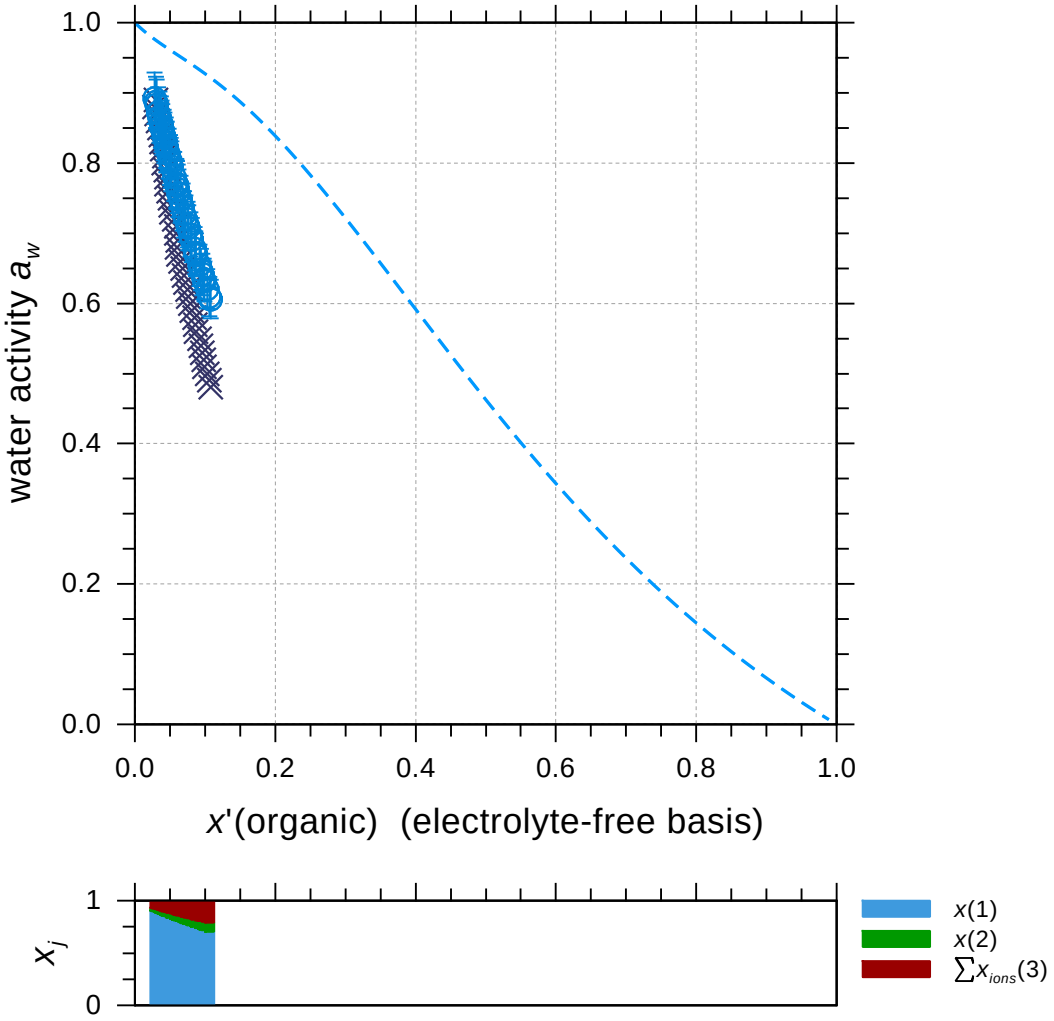


initial weighting of dataset:
$w^{init}(0387)$ = 2.000
dataset contribution to F_{obj}:
fval(0387) = 1.2736E-03
rel. contribution = 0.0006 %

Fig. S0261 (AIOMFAC_output_0958)

H_2O (1) + Glutaric_acid (2) + NaCl (3)

Temperature: 295 K

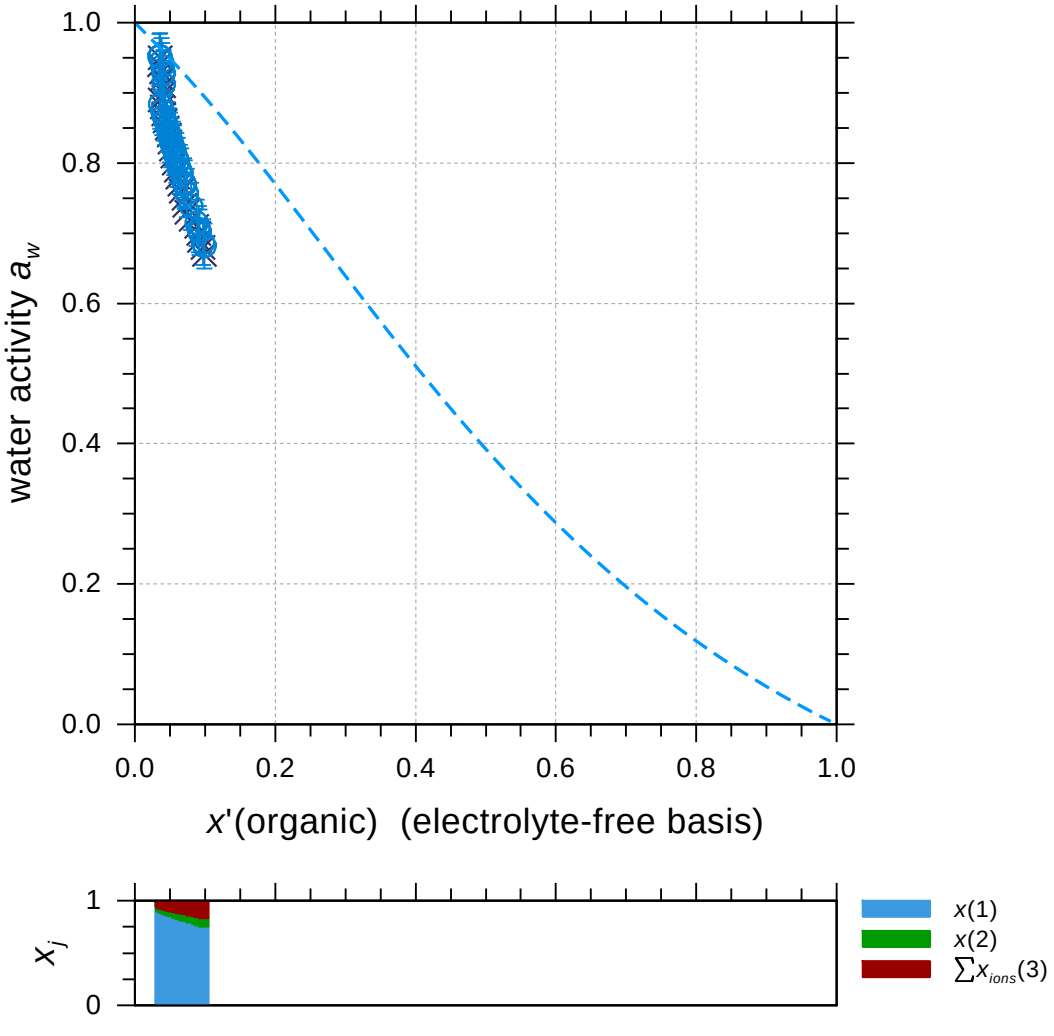


initial weighting of dataset:
$w^{init}(0958)$ = 1.000
dataset contribution to F_{obj}:
fval(0958) = 1.7131E-01
rel. contribution = 0.0815 %

Fig. S0262 (AIOMFAC_output_0959)

H_2O (1) + Malonic_acid (2) + NaCl (3)

Temperature: 295 K

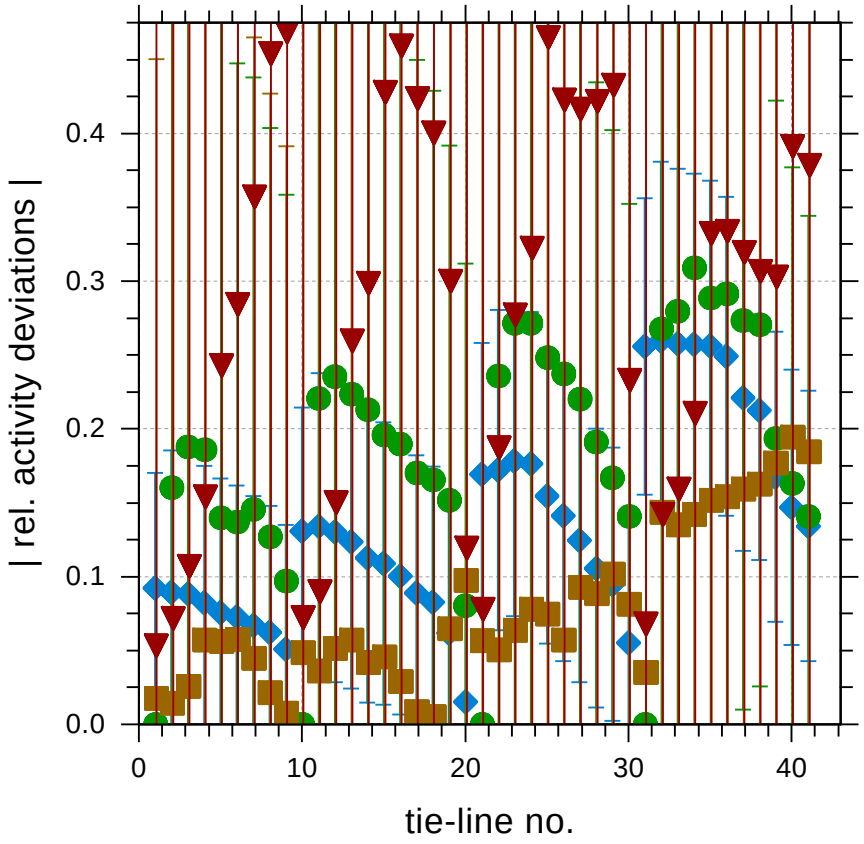


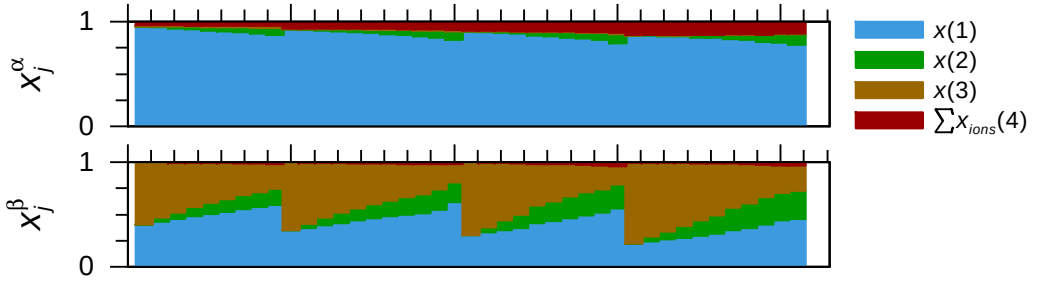
initial weighting of dataset:
$w^{init}(0959)$ = 1.000
dataset contribution to F_{obj}:
fval(0959) = 3.4013E-03
rel. contribution = 0.0016 %

Fig. S0263 (AIOMFAC_output_0932)

H_2O (1) + Acetic_acid (2) + 1-Butanol (3) + NaCl (4)

Temperature: 298 K



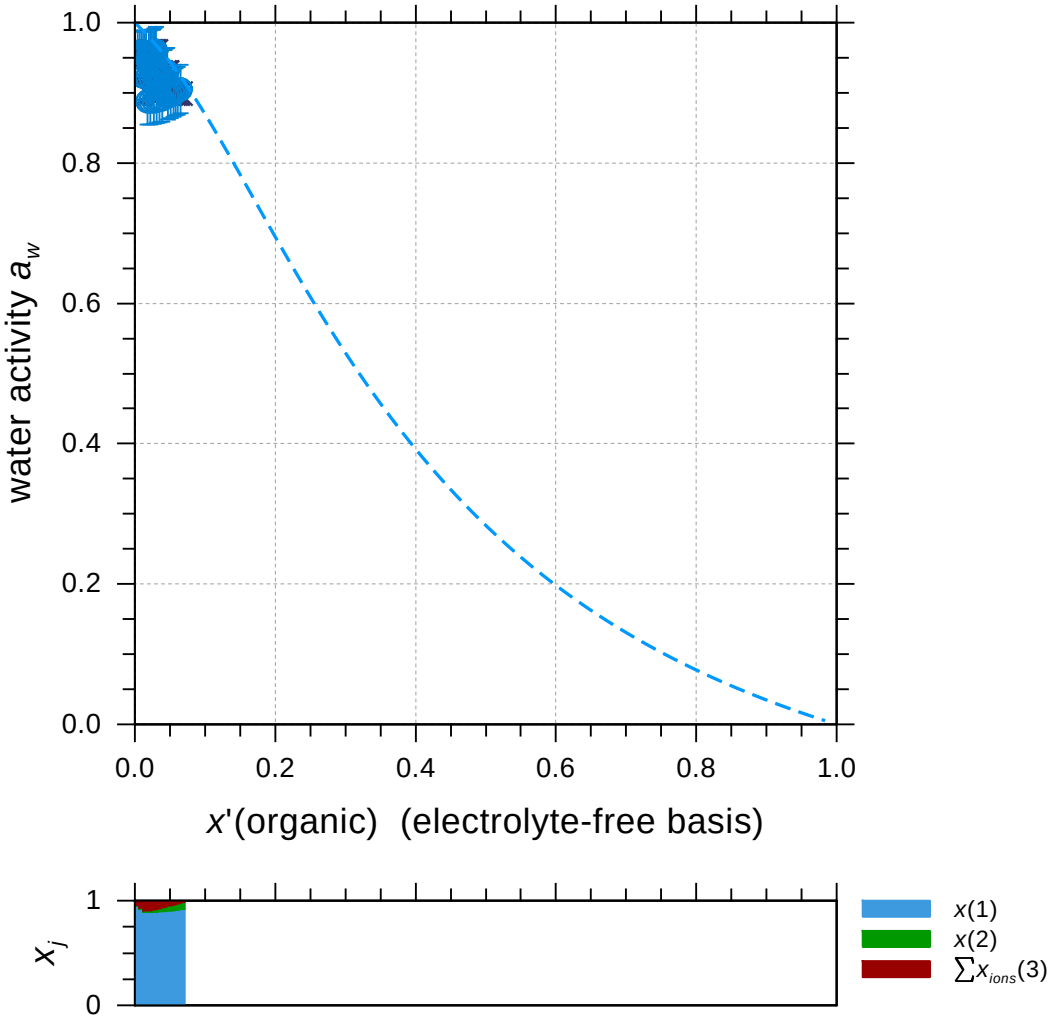


initial weighting of dataset:
$w^{init}(0932)$ = 1.000
dataset contribution to F_{obj}:
fval(0932) = 8.3059E-01
rel. contribution = 0.3950 %

Fig. S0264 (AIOMFAC_output_0301)

H_2O (1) + Citric_acid (2) + $NaNO_3$ (3)

Temperature: 298 K

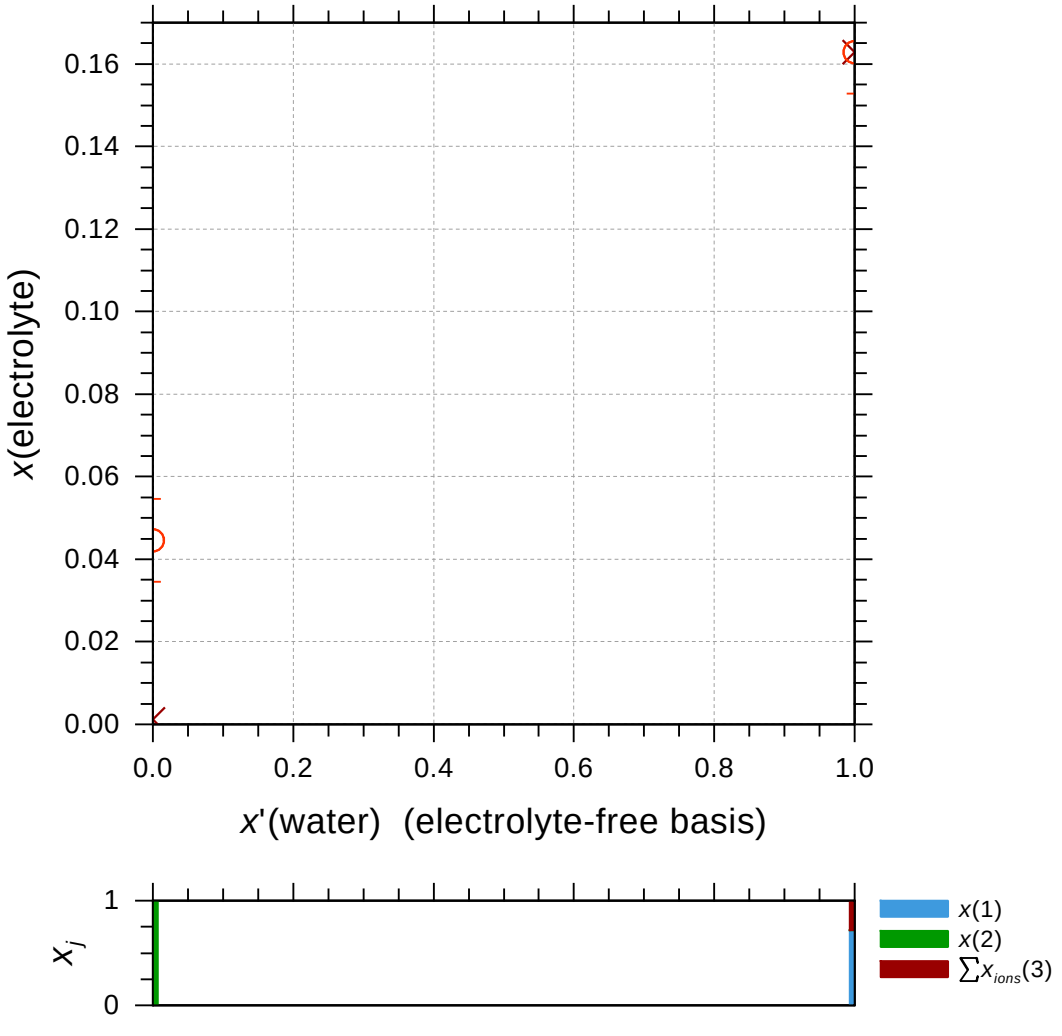


initial weighting of dataset:
w^{init}(0301) = 2.000
dataset contribution to F_{obj}:
fval(0301) = 5.8517E-04
rel. contribution = 0.0003 %

Fig. S0265 (AIOMFAC_output_0940)

H_2O (1) + Acetic_acid (2) + $NaNO_3$ (3)

Temperature: 298 K

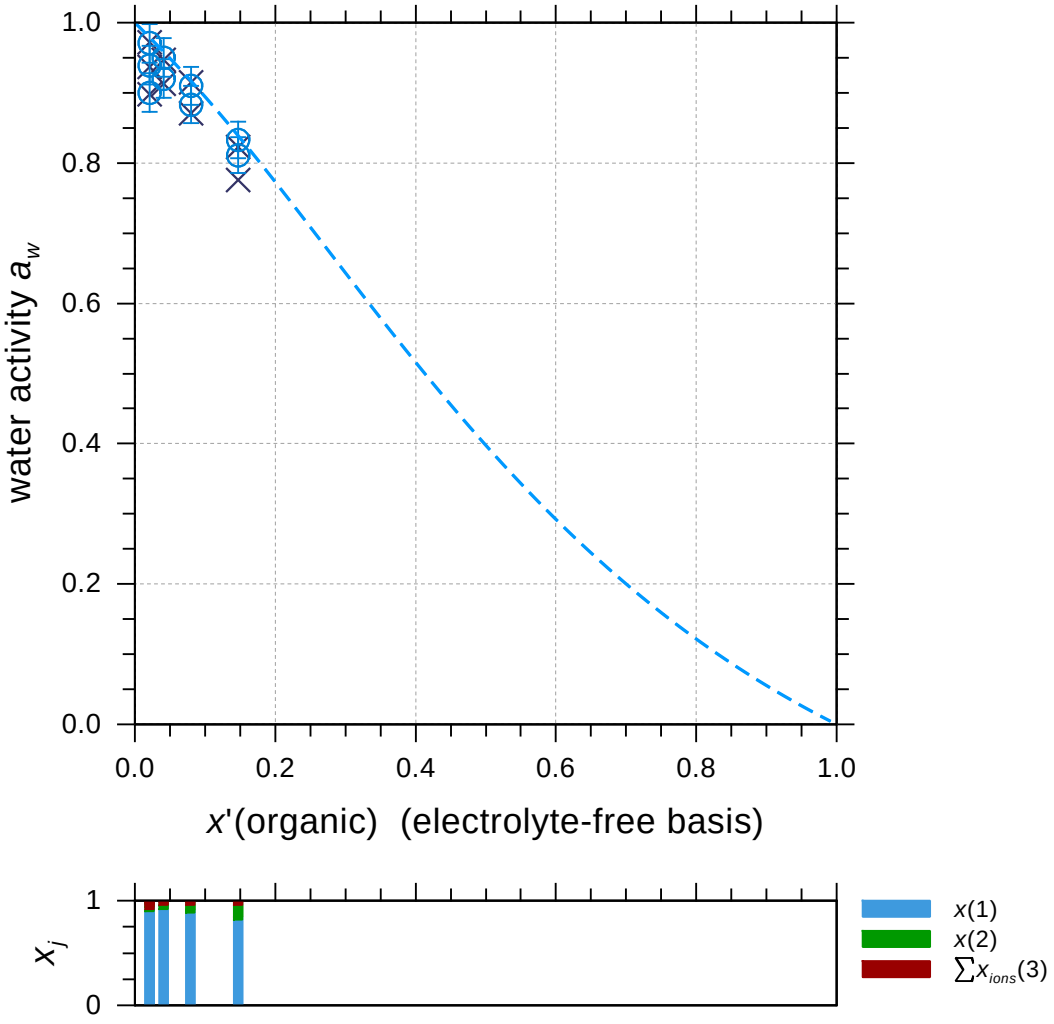


initial weighting of dataset:
$w^{init}(0940)$ = 0.010
dataset contribution to F_{obj}:
fval(0940) = 1.4992E-01
rel. contribution = 0.0713 %

Fig. S0266 (AIOMFAC_output_0390)

H_2O (1) + Malonic_acid (2) + NH_4Br (3)

Temperature: 303 K

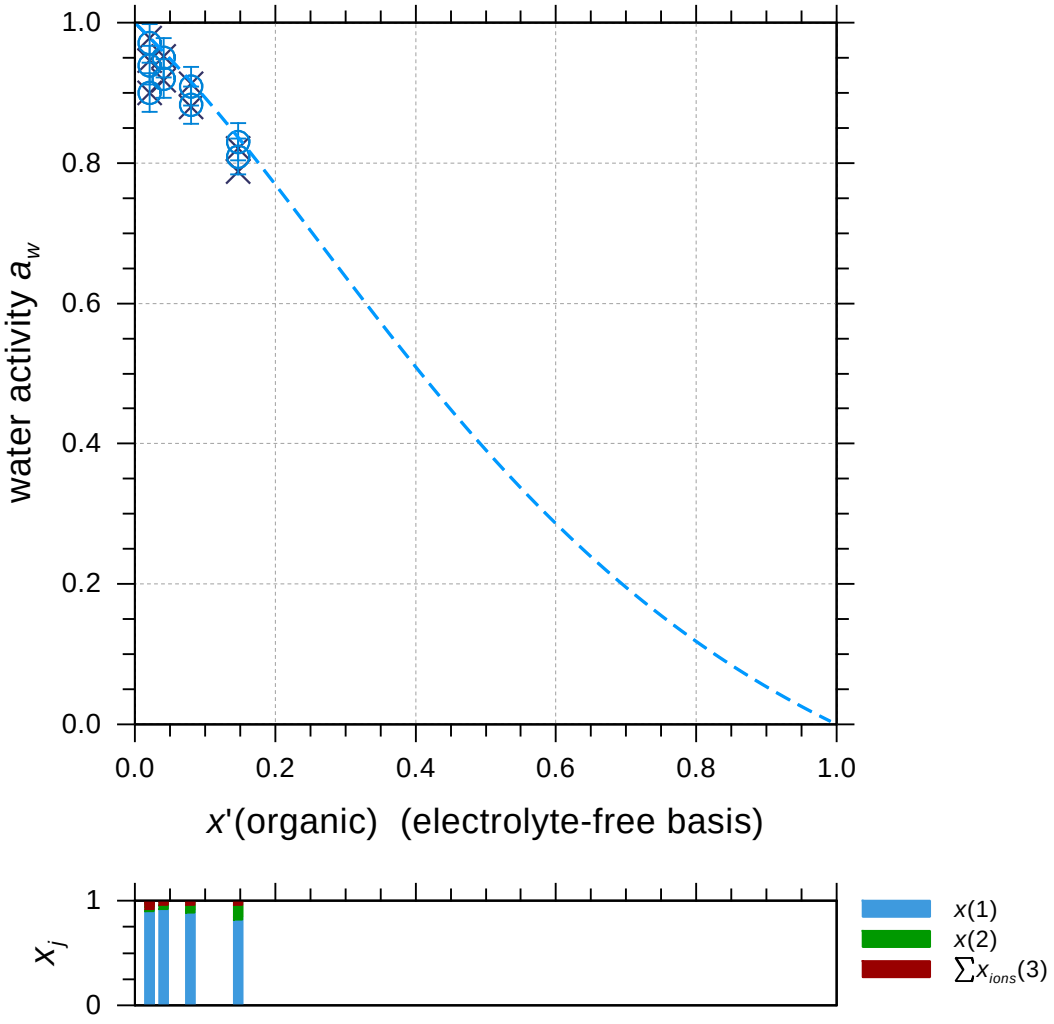


initial weighting of dataset:
$w^{init}(0390)$ = 2.000
dataset contribution to F_{obj}:
fval(0390) = 4.7264E-03
rel. contribution = 0.0022 %

Fig. S0267 (AIOMFAC_output_0391)

H_2O (1) + Malonic_acid (2) + NH_4Br (3)

Temperature: 293 K

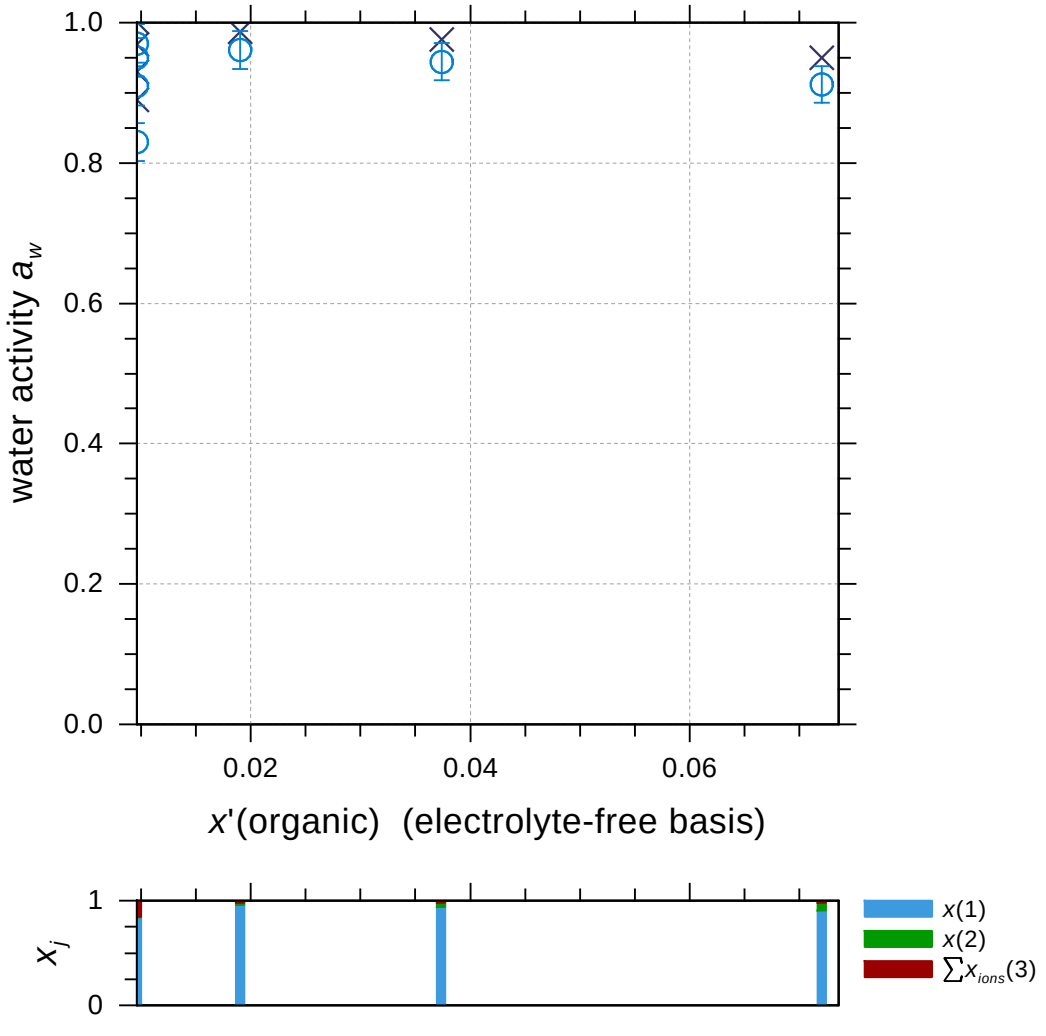


initial weighting of dataset:
w^{init}(0391) = 2.000
dataset contribution to F_{obj}:
fval(0391) = 1.8403E-03
rel. contribution = 0.0009 %

Fig. S0268 (AIOMFAC_output_0970)

H_2O (1) + Maleic_acid (2) + NH_4Br (3)

Temperature: 293 K

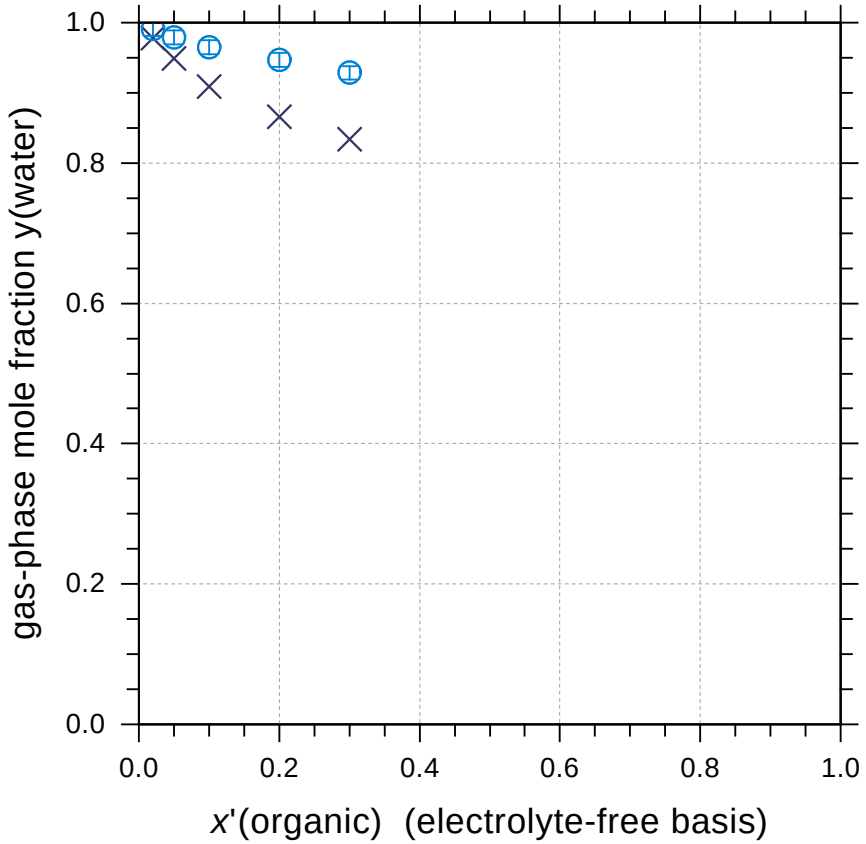


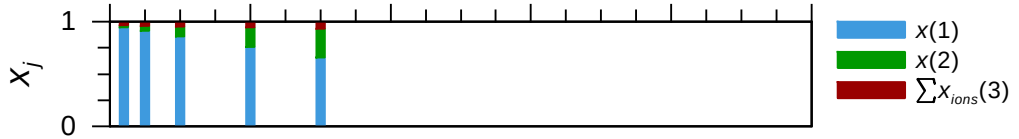
initial weighting of dataset:
$w^{init}(0970)$ = 2.000
dataset contribution to F_{obj}:
fval(0970) = 1.8369E-02
rel. contribution = 0.0087 %

Fig. S0269 (AIOMFAC_output_0333)

H_2O (1) + Propanoic_acid (2) + NH_4Cl (3)

Temperature: 333 K





left y-axis:

× NH4Cl+PropanoicAcid+Water_VLE_Banat_333K

○ AIOMFAC gas-phase composition y(water)

initial weighting of dataset:

$w^{init}(0333)$ = 0.500

dataset contribution to F_{obj}:

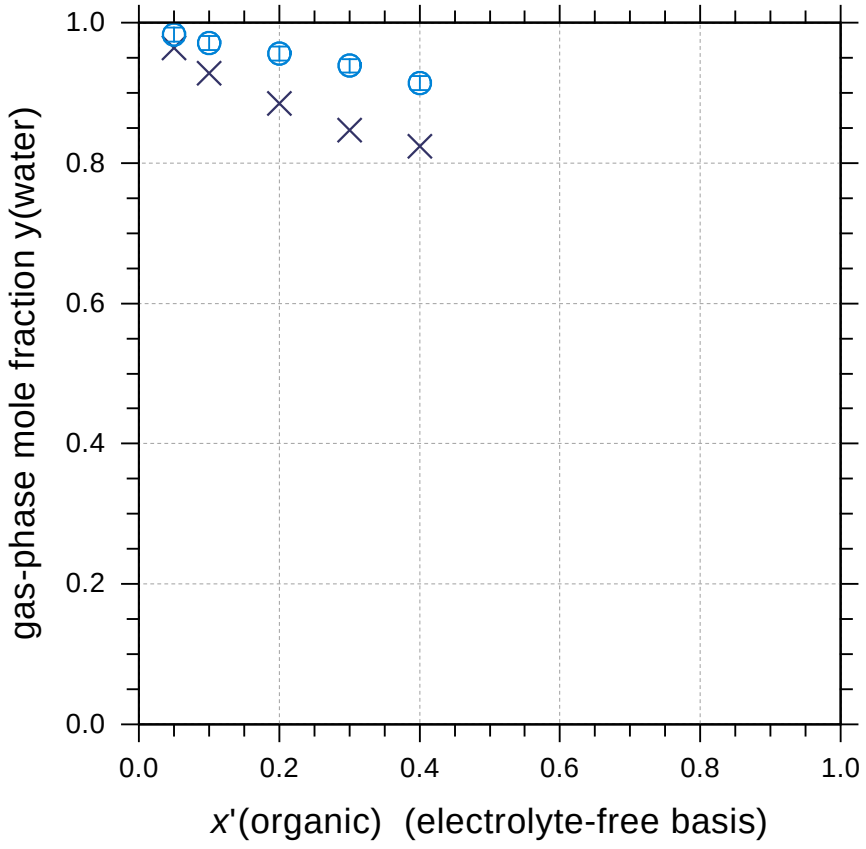
fval(0333) = 1.2900E-02

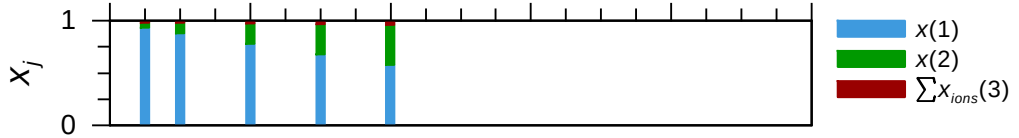
rel. contribution = 0.0061 %

Fig. S0270 (AIOMFAC_output_0340)

H_2O (1) + Propanoic_acid (2) + NH_4Cl (3)

Temperature: 313 K





left y-axis:

× NH4Cl+PropanoicAcid+Water_VLE_Banat_313K

○ AIOMFAC gas-phase composition y(water)

initial weighting of dataset:

$w^{init}(0340)$ = 0.500

dataset contribution to F_{obj}:

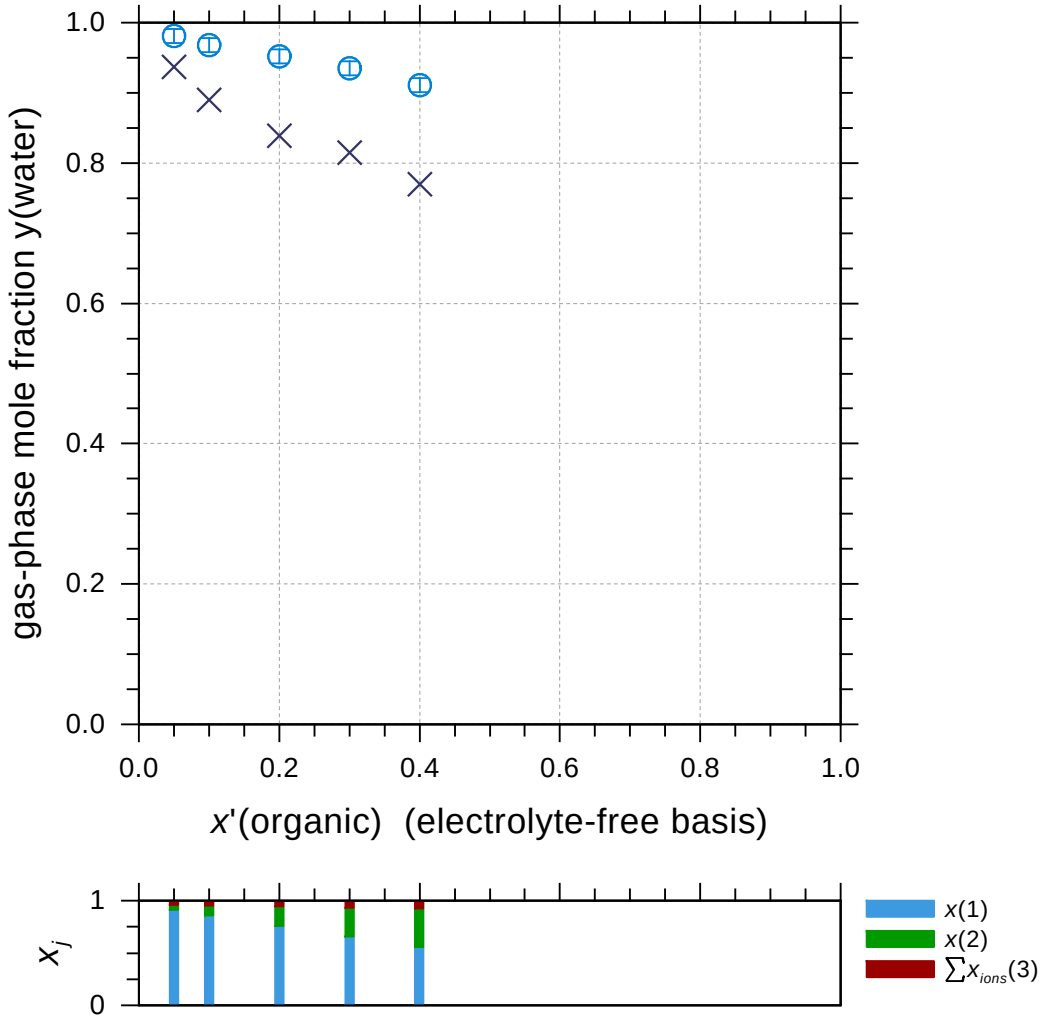
fval(0340) = 1.5864E-02

rel. contribution = 0.0075 %

Fig. S0271 (AIOMFAC_output_0341)

H_2O (1) + Propanoic_acid (2) + NH_4Cl (3)

Temperature: 323 K



initial weighting of dataset:
$w^{init}(0341)$ = 0.500
dataset contribution to F_{obj}:
fval(0341) = 4.0326E-02
rel. contribution = 0.0192 %

Fig. S0272 (AIOMFAC_output_1052)

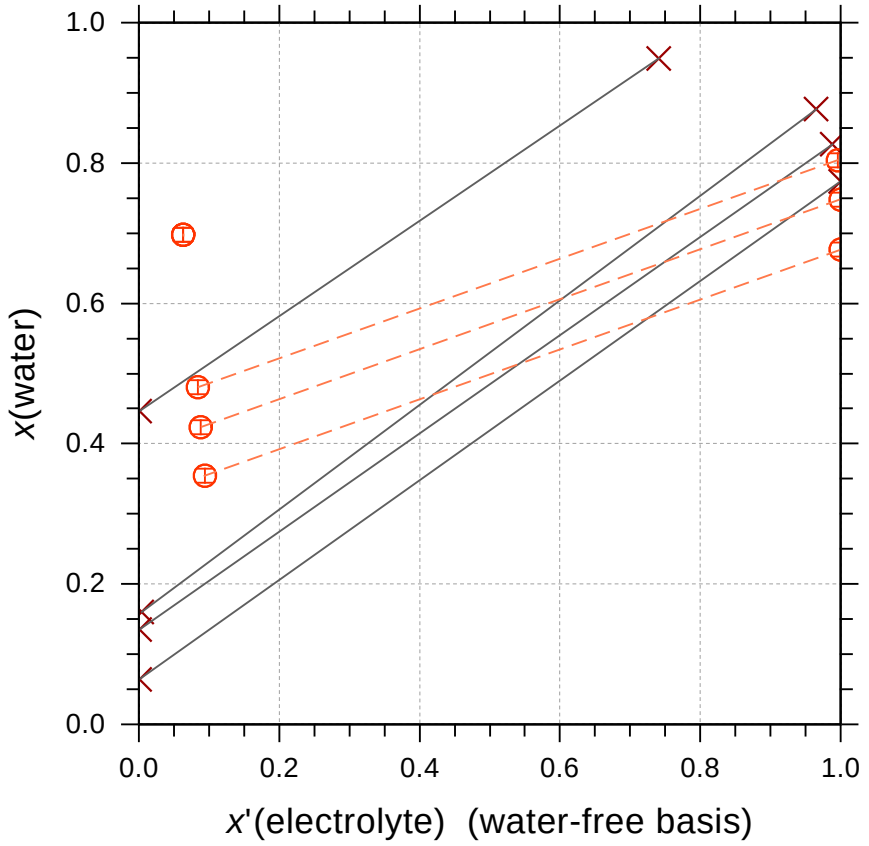
H_2O (1) + Methacrylic_acid (2) + NH_4HSO_4 (3)

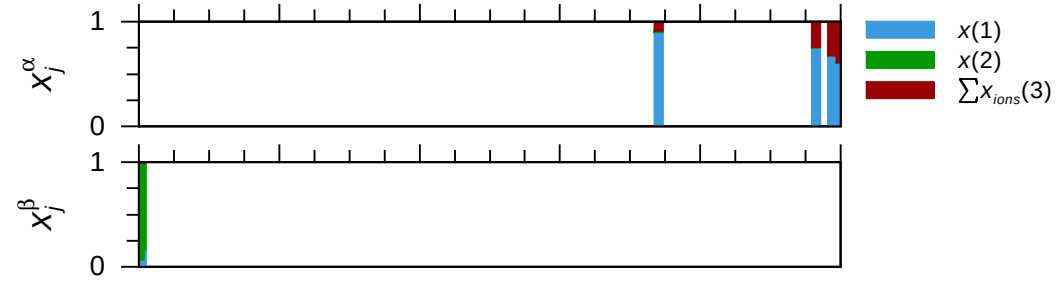
Temperature: 298 K

left y-axis:

× NH4HSO4+MethacrylicAcid+Water_LLE_Obmelyukhina

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(1052) = 0.010

dataset contribution to F_{obj}:

fval(1052) = 3.4664E-02

rel. contribution = 0.0165 %

Fig. S0272a (AIOMFAC_output_1052)

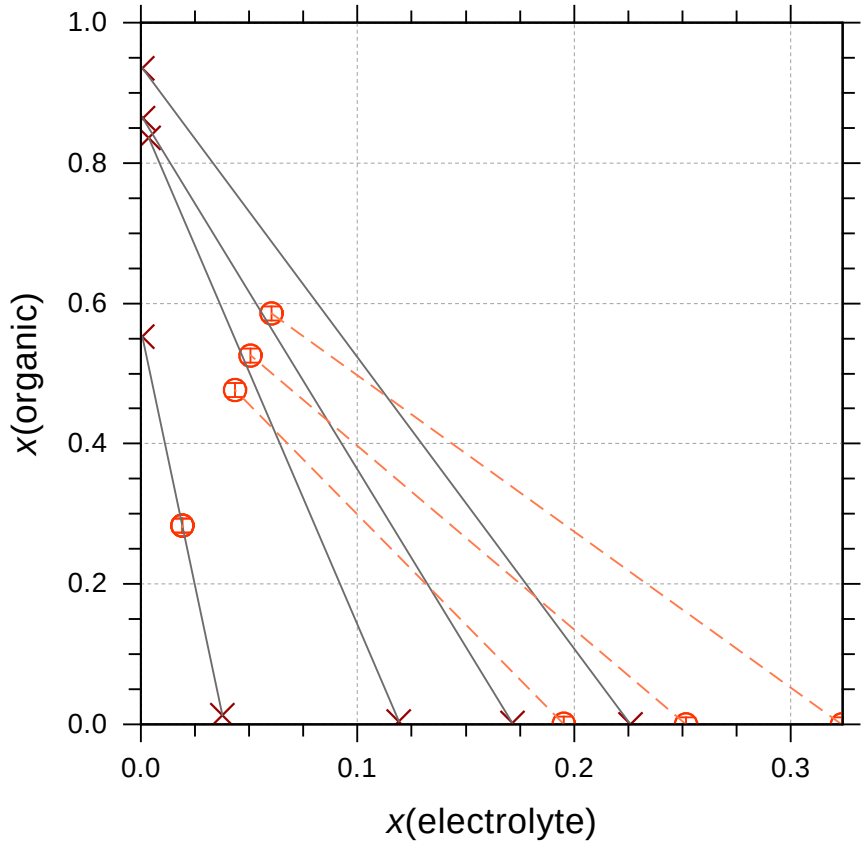
H_2O (1) + Methacrylic_acid (2) + NH_4HSO_4 (3)

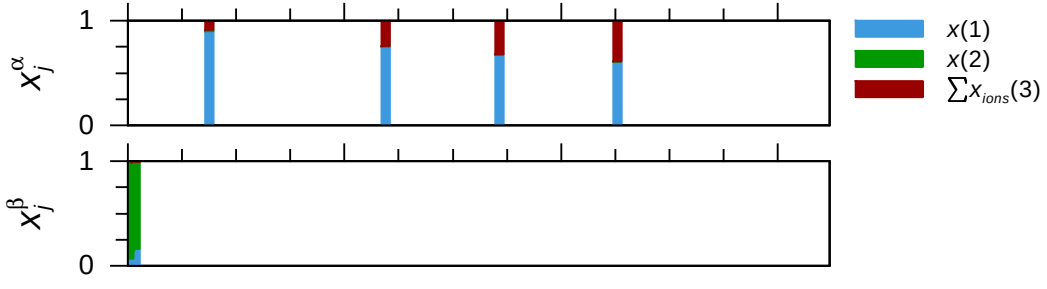
Temperature: 298 K

left y-axis:

× NH4HSO4+MethacrylicAcid+Water_LLE_Obmelyukhina

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(1052)$ = 0.010

dataset contribution to F_{obj}:

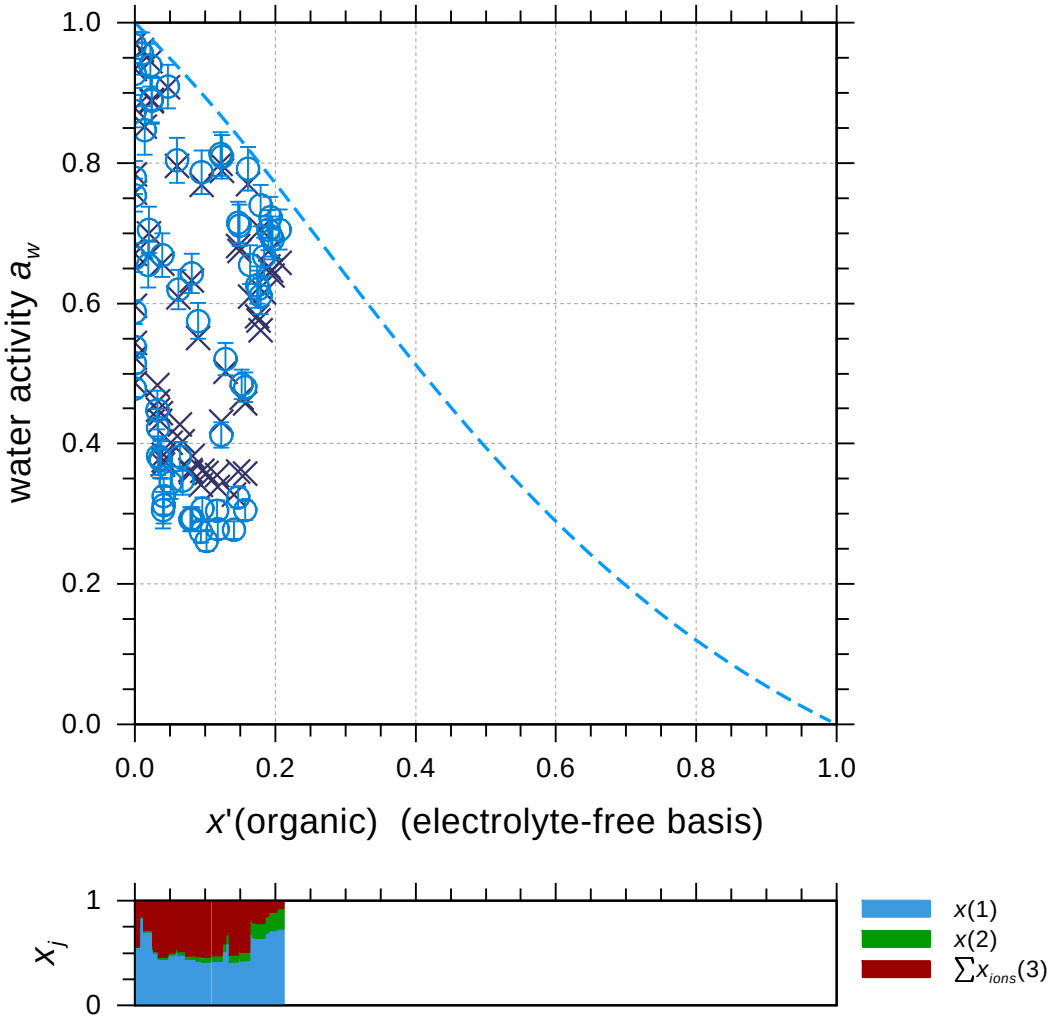
fval(1052) = 3.4664E-02

rel. contribution = 0.0165 %

Fig. S0273 (AIOMFAC_output_0272)

H_2O (1) + Malonic_acid (2) + NH_4HSO_4 (3)

Temperature: 298 K

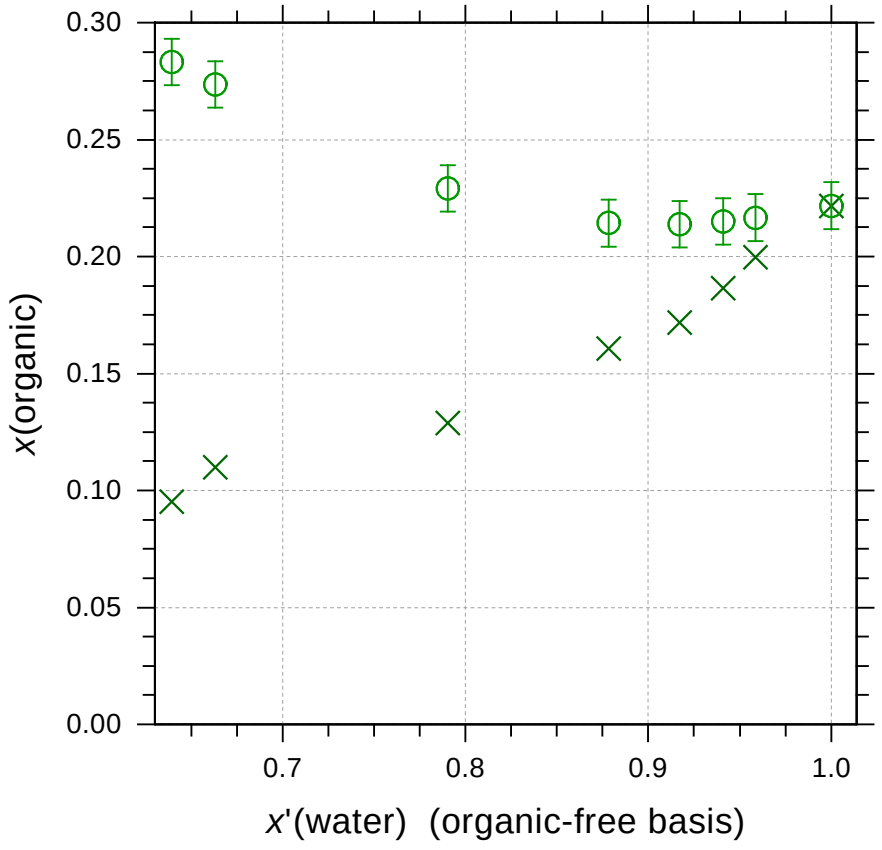


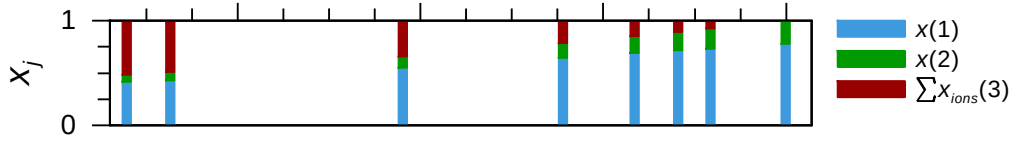
initial weighting of dataset:
w^{init}(0272) = 2.000
dataset contribution to F_{obj}:
fval(0272) = 1.7932E-01
rel. contribution = 0.0853 %

Fig. S0274 (AIOMFAC_output_0273)

H_2O (1) + Malonic_acid (2) + NH_4HSO_4 (3)

Temperature: 298 K





left y-axis:

× NH4HSO4+MalonicAcid+Water_SLE-org_Salcedo

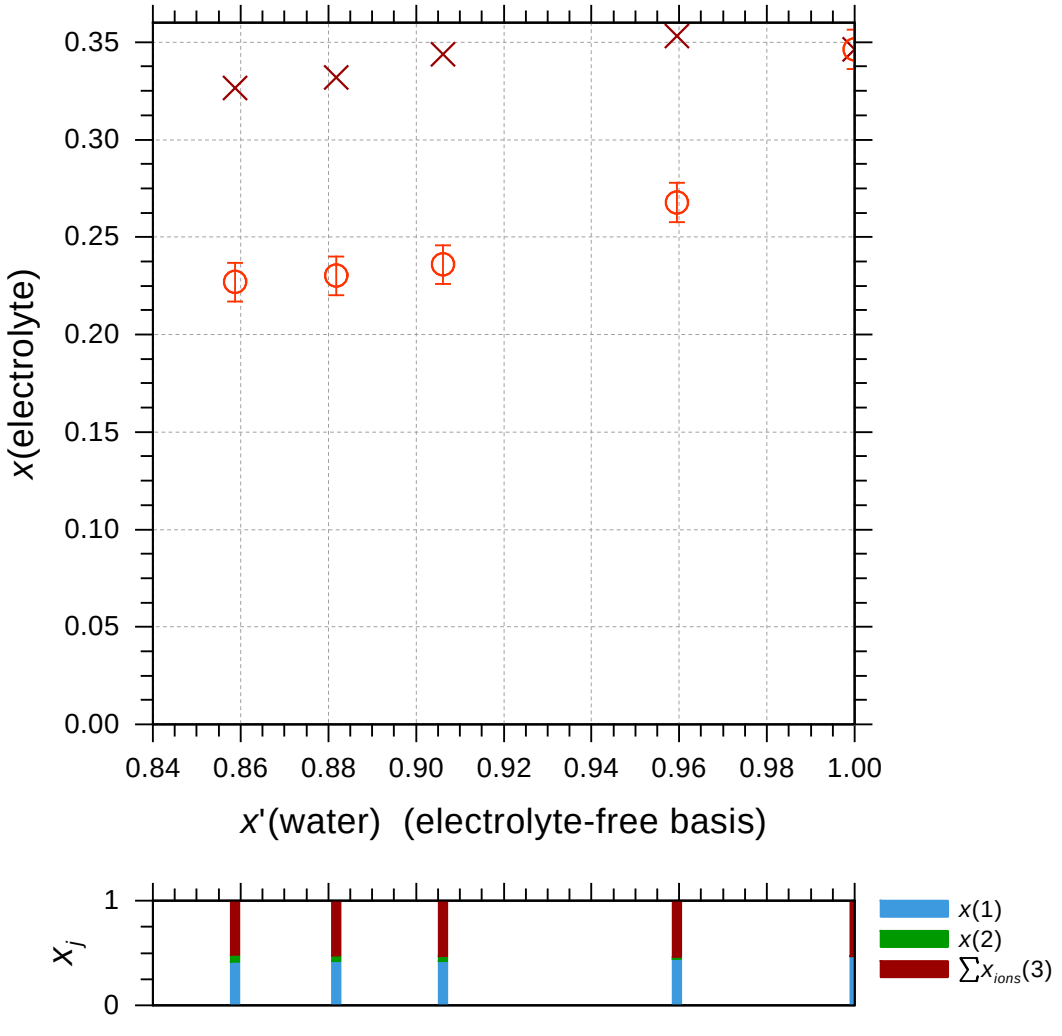
○ AIOMFAC calc. SLE composition

initial weighting of dataset:
w^{init}(0273) = 1.000
dataset contribution to F_{obj}:
fval(0273) = 5.9522E+00
rel. contribution = 2.8305 %

Fig. S0275 (AIOMFAC_output_0274)

H_2O (1) + Malonic_acid (2) + NH_4HSO_4 (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0274)$ = 1.000

dataset contribution to F_{obj}:

fval(0274) = 4.7635E-01

rel. contribution = 0.2265 %

left y-axis:

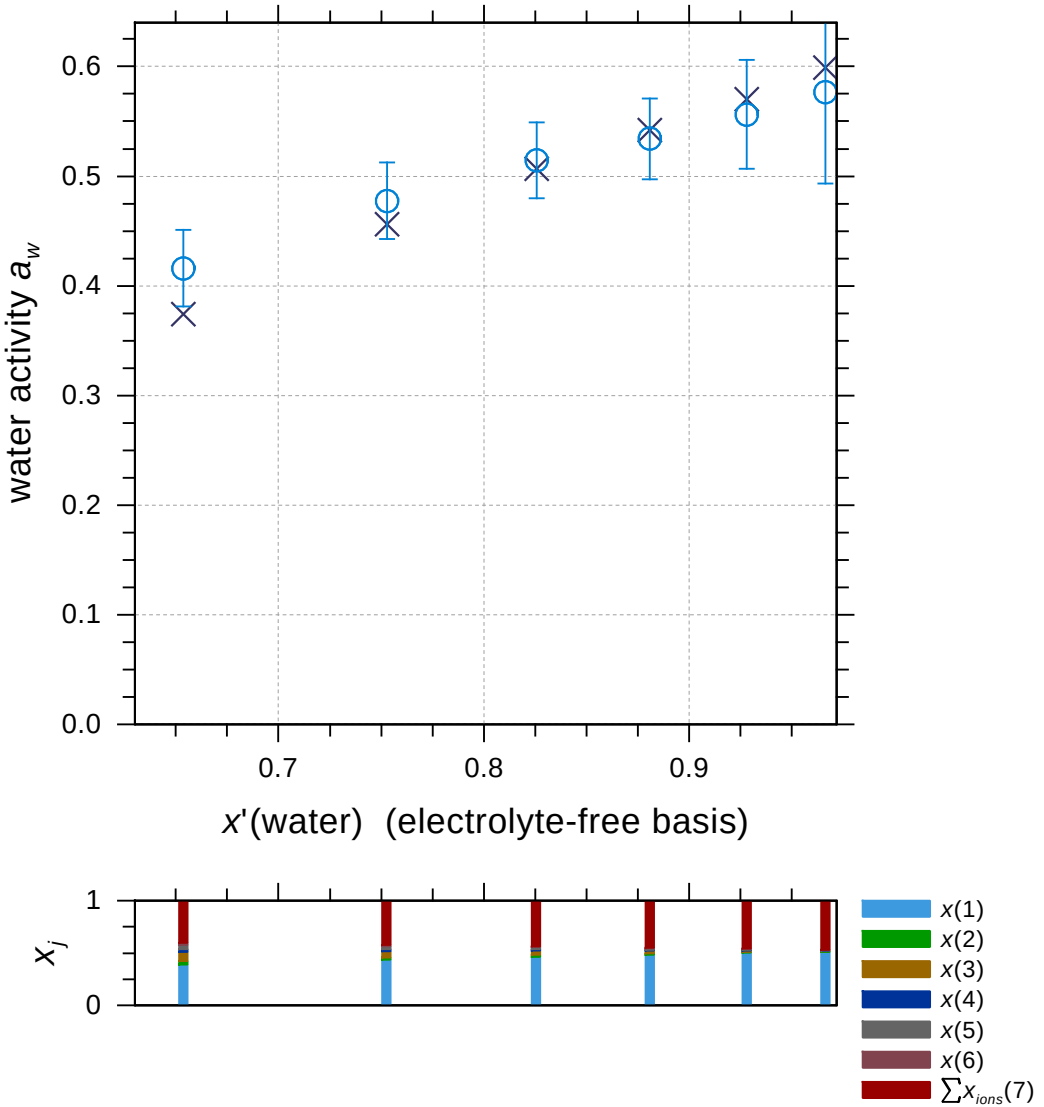
× NH4NO3+DicarboxylicAcidsMixtureM5+Water_aw_Marcolli

○ AIOMFAC water activity a_w

Fig. S0276 (AIOMFAC_output_0288)

H_2O (1) + Malic_acid (2) + Malonic_acid (3) + Maleic_acid (4) + Glutaric_acid (5) + Methylsuccinic_acid (6) + NH_4NO_3 (7)

Temperature: 298 K



initial weighting of dataset:

w^{init}(0288) = 2.000

dataset contribution to F_{obj}:

fval(0288) = 2.8847E-02

rel. contribution = 0.0137 %

left y-axis:

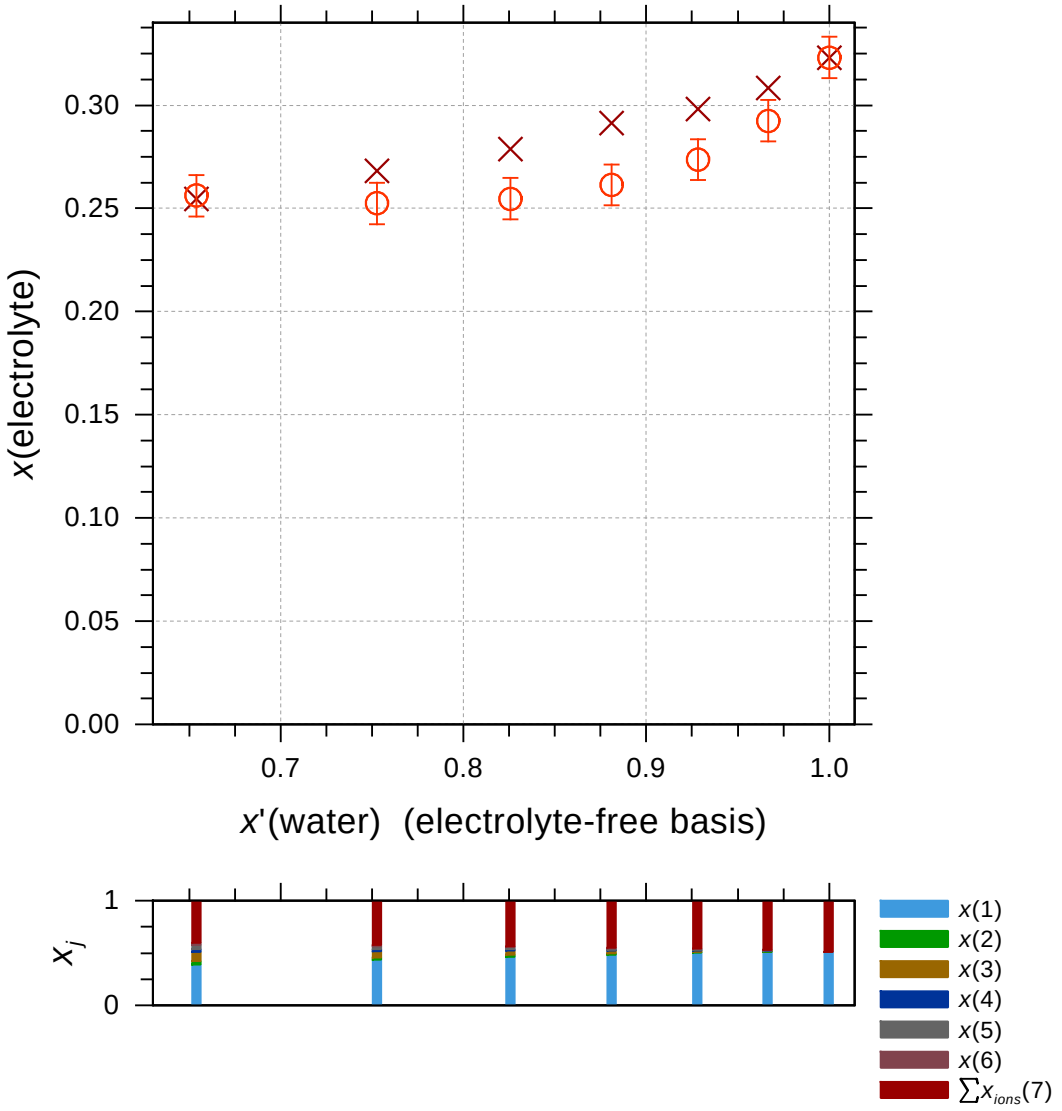
× NH4NO3+DicarboxylicAcidsMixtureM5+Water_SLE-salt_Marcolli

○ AIOMFAC calc. SLE composition

Fig. S0277 (AIOMFAC_output_0289)

H_2O (1) + Malic_acid (2) + Malonic_acid (3) + Maleic_acid (4) + Glutaric_acid (5) + Methylsuccinic_acid (6) + NH_4NO_3 (7)

Temperature: 298 K



initial weighting of dataset:

w^{init}(0289) = 1.000

dataset contribution to F_{obj}:

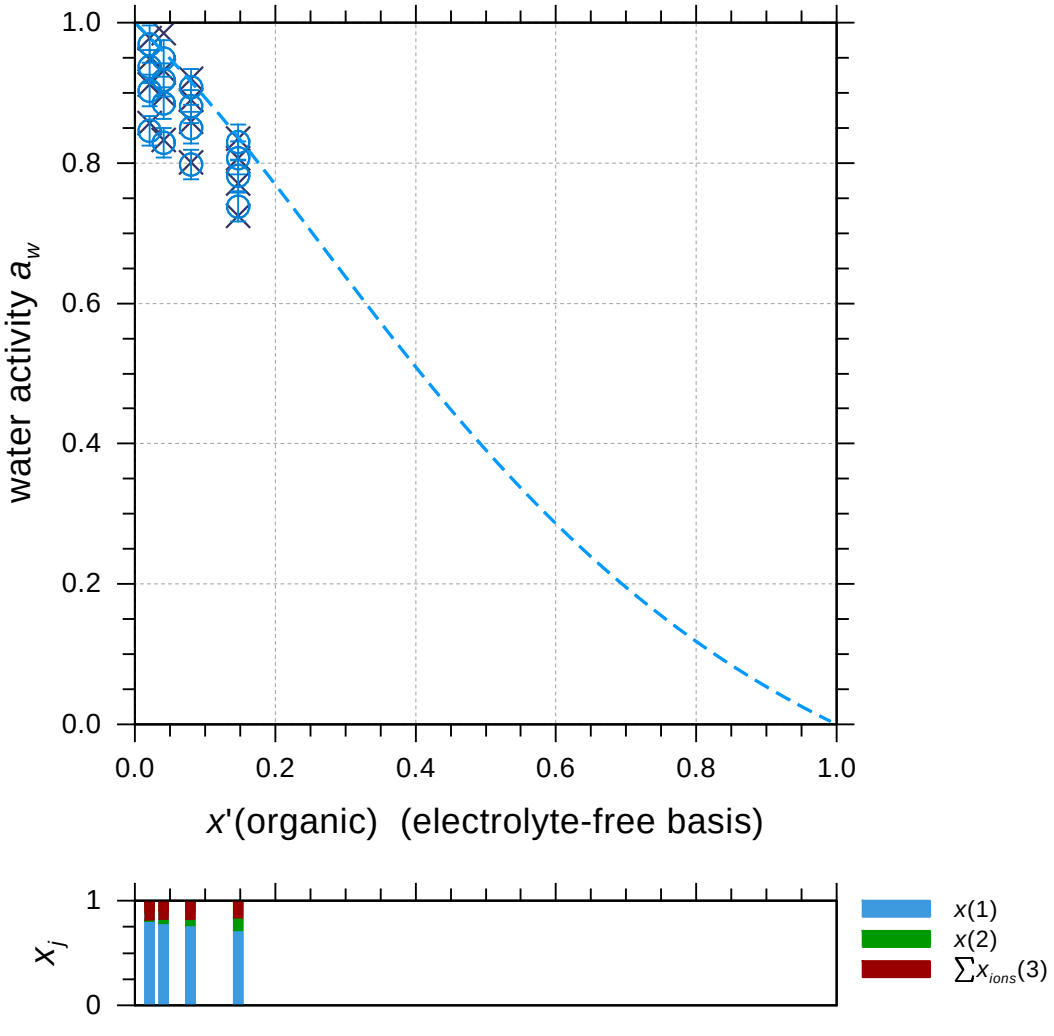
fval(0289) = 4.2440E-02

rel. contribution = 0.0202 %

Fig. S0278 (AIOMFAC_output_0382)

H_2O (1) + Malonic_acid (2) + NH_4NO_3 (3)

Temperature: 293 K

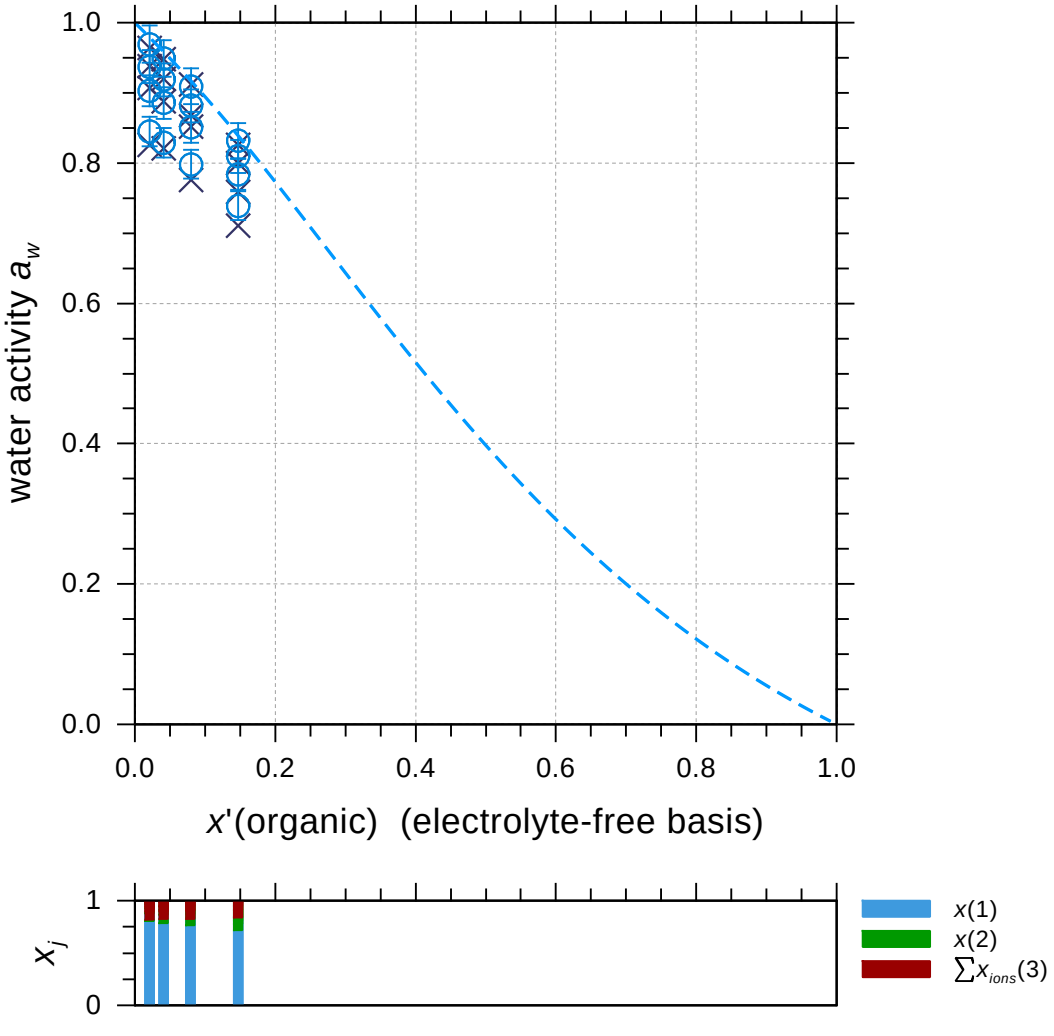


initial weighting of dataset:
$w^{init}(0382)$ = 2.000
dataset contribution to F_{obj}:
fval(0382) = 3.7377E-03
rel. contribution = 0.0018 %

Fig. S0279 (AIOMFAC_output_0383)

H_2O (1) + Malonic_acid (2) + NH_4NO_3 (3)

Temperature: 303 K

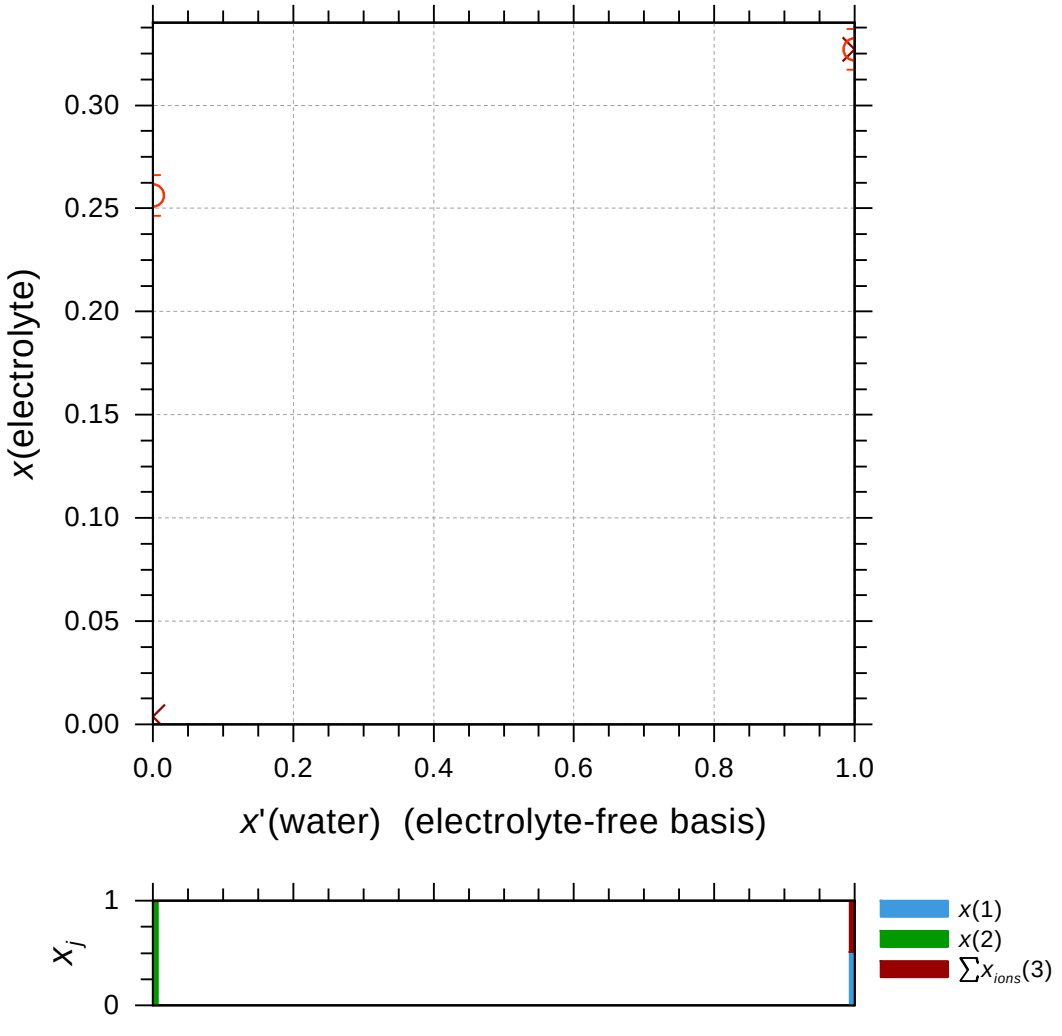


initial weighting of dataset:
$w^{init}(0383)$ = 2.000
dataset contribution to F_{obj}:
fval(0383) = 5.4510E-03
rel. contribution = 0.0026 %

Fig. S0280 (AIOMFAC_output_0942)

H_2O (1) + Acetic_acid (2) + NH_4NO_3 (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0942)$ = 0.010

dataset contribution to F_{obj}:

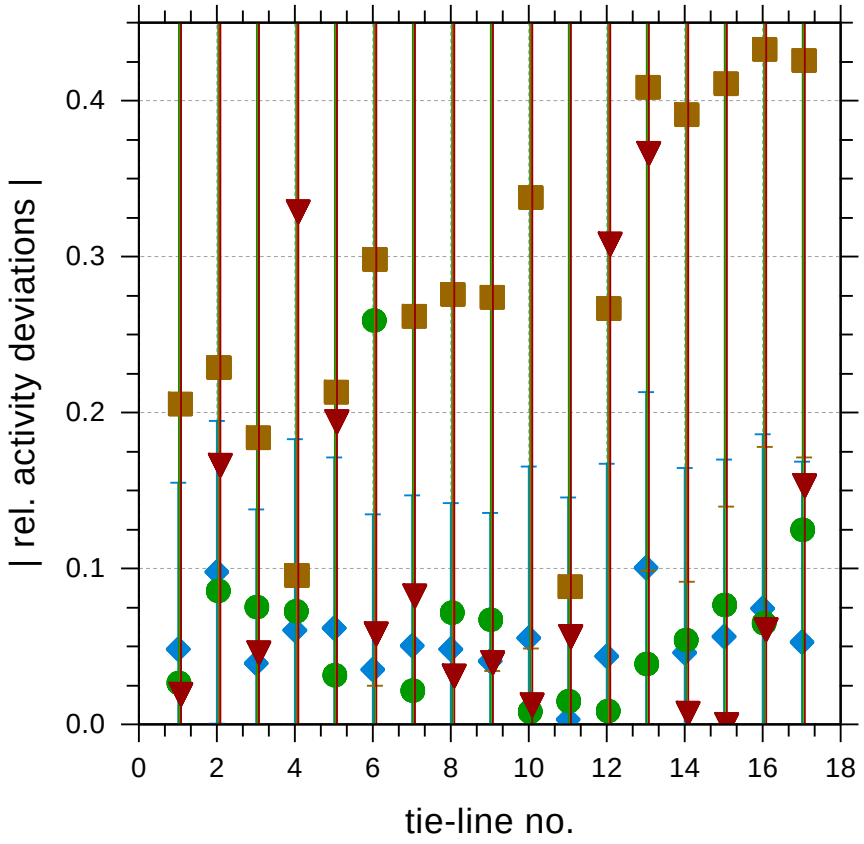
fval(0942) = 3.4004E+00

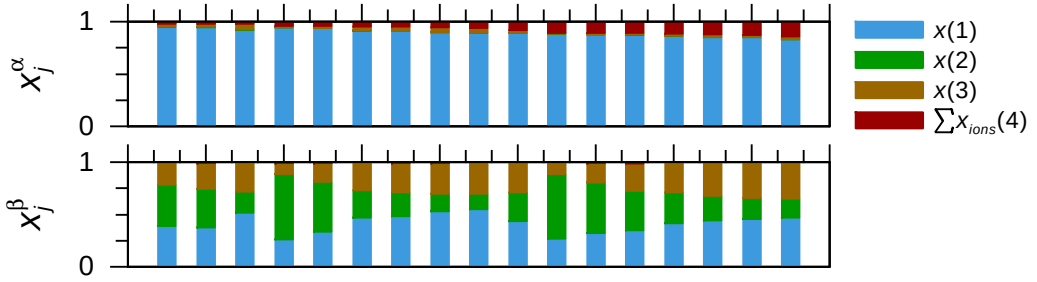
rel. contribution = 1.6170 %

Fig. S0281 (AIOMFAC_output_0305)

H_2O (1) + 4-Methyl-2-pentanone (2) + Propanoic_acid (3) + $(NH_4)_2SO_4$ (4)

Temperature: 308 K





left y-axis:

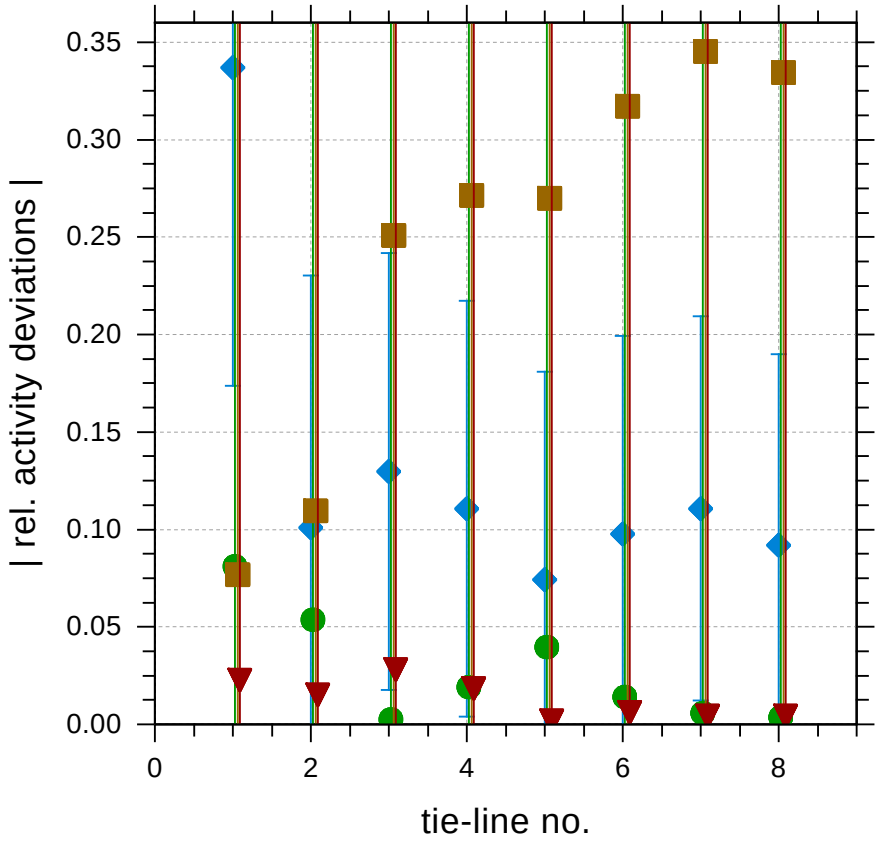
- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

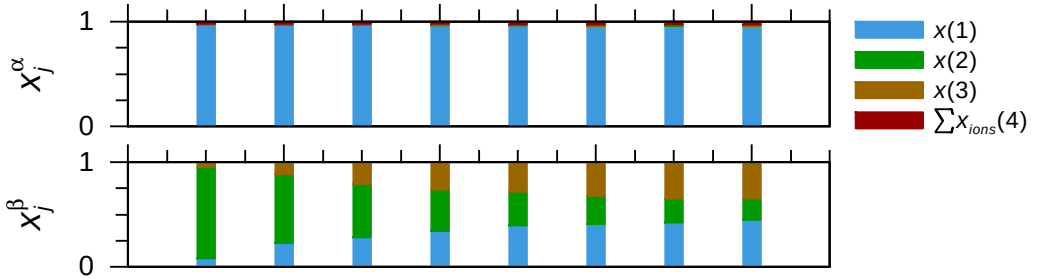
initial weighting of dataset:
$w^{init}(0305)$ = 1.000
dataset contribution to F_{obj}:
fval(0305) = 6.3967E-01
rel. contribution = 0.3042 %

Fig. S0282 (AIOMFAC_output_0309)

H_2O (1) + 4-Methyl-2-pentanone (2) + Butyric_acid (3) + $(NH_4)_2SO_4$ (4)

Temperature: 308 K





initial weighting of dataset:

w^{init}(0309) = 1.000

dataset contribution to F_{obj}:

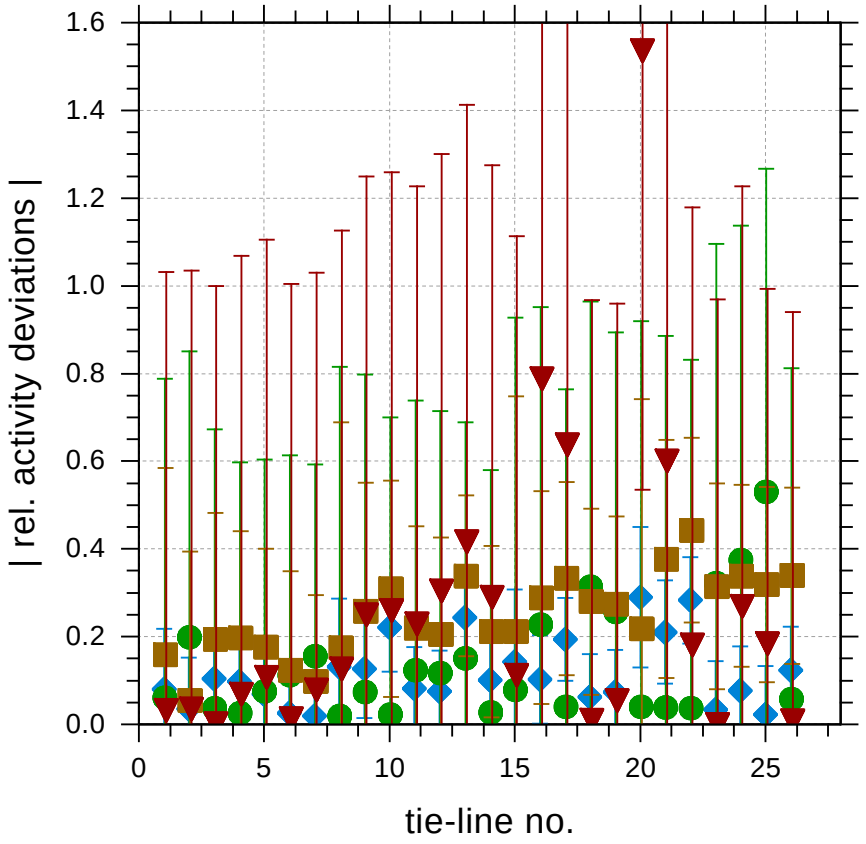
fval(0309) = 4.7581E-01

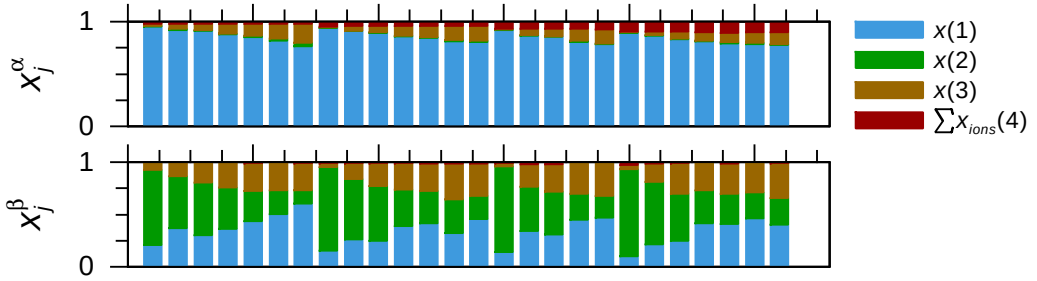
rel. contribution = 0.2263 %

Fig. S0283 (AIOMFAC_output_0316)

H_2O (1) + 4-Methyl-2-pentanone (2) + Acetic_acid (3) + $(NH_4)_2SO_4$ (4)

Temperature: 308 K





left y-axis:

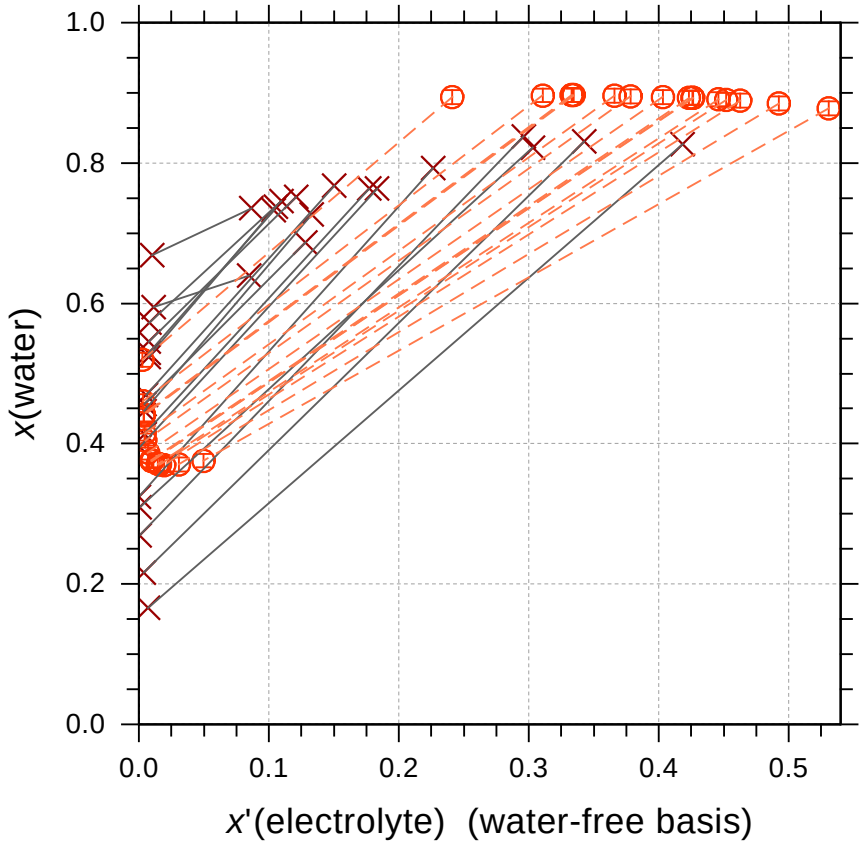
- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

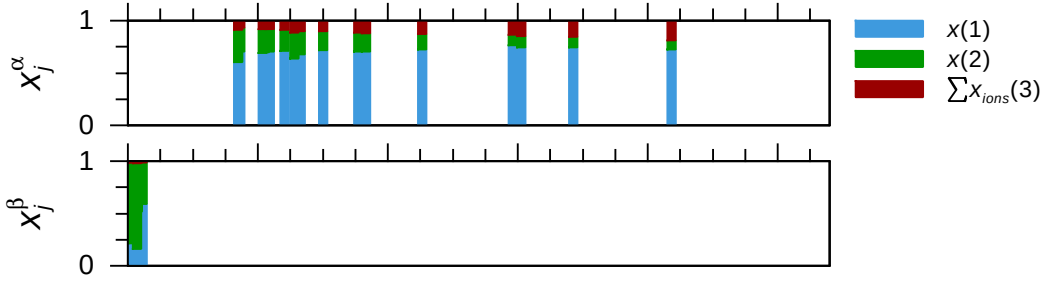
initial weighting of dataset:
w^{init}(0316) = 1.000
dataset contribution to F_{obj}:
fval(0316) = 1.4796E+00
rel. contribution = 0.7036 %

Fig. S0284 (AIOMFAC_output_1050)

H_2O (1) + Acetone (2) + $CaCl_2$ (3)

Temperature: 296 K





left y-axis:

× CaCl2+Acetone+Water_LLE_Bourayou_1

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1050) = 1.000

dataset contribution to F_{obj}:

fval(1050) = 1.0964E+00

rel. contribution = 0.5214 %

Fig. S0284a (AIOMFAC_output_1050)

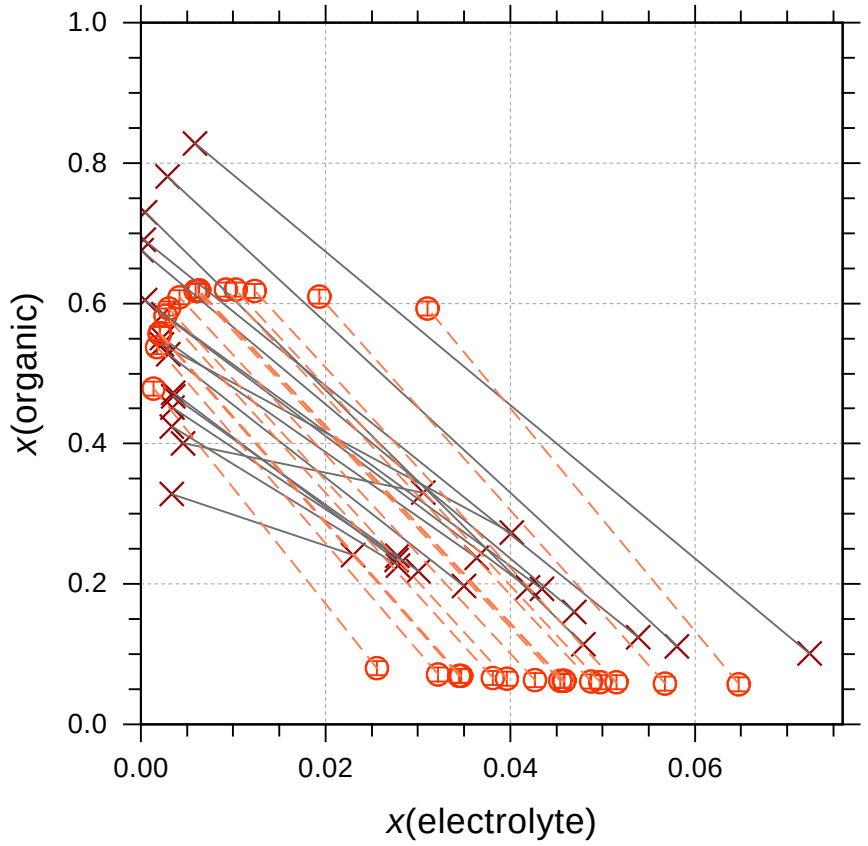
H_2O (1) + Acetone (2) + $CaCl_2$ (3)

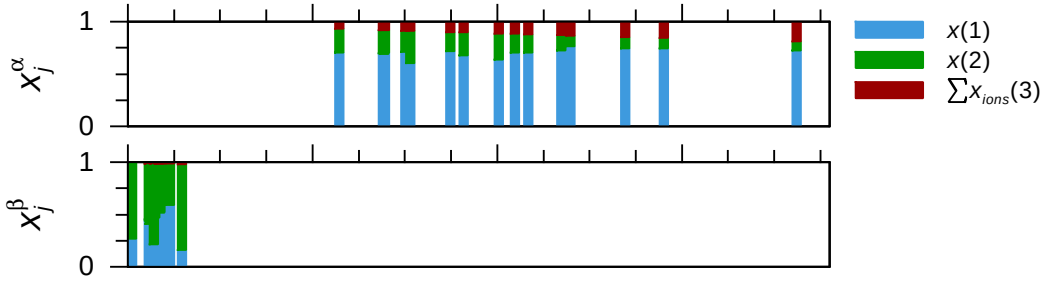
Temperature: 296 K

left y-axis:

× CaCl2+Acetone+Water_LLE_Bourayou_1

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(1050)$ = 1.000

dataset contribution to F_{obj}:

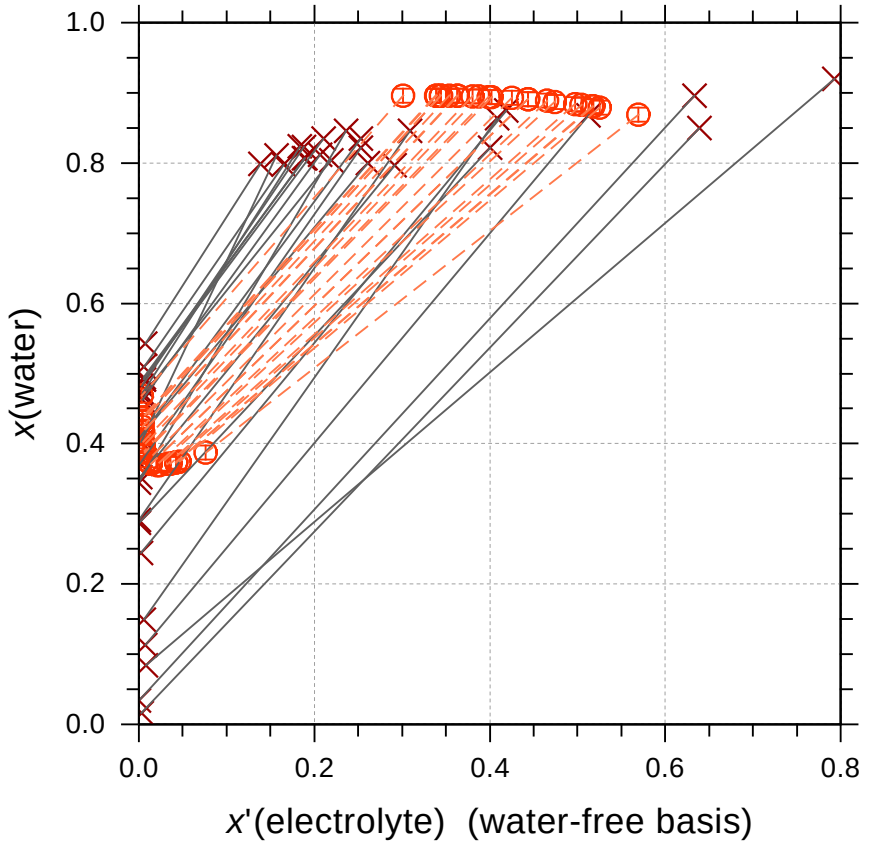
fval(1050) = 1.0964E+00

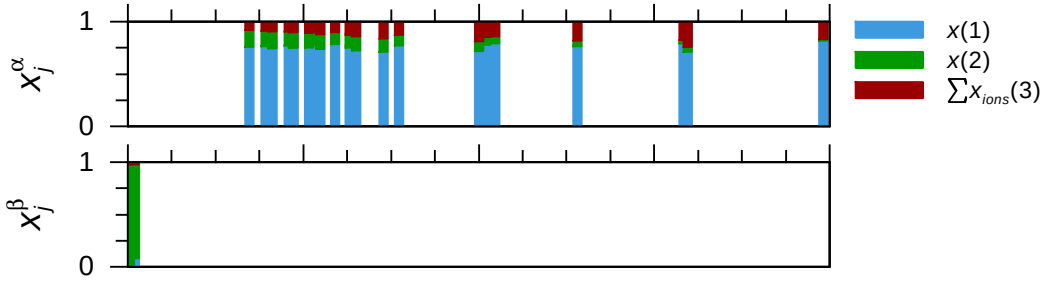
rel. contribution = 0.5214 %

Fig. S0285 (AIOMFAC_output_1051)

H_2O (1) + Acetone (2) + $CaCl_2$ (3)

Temperature: 296 K





left y-axis:

× CaCl2+Acetone+Water_LLE_Bourayou_2

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1051) = 1.000

dataset contribution to F_{obj}:

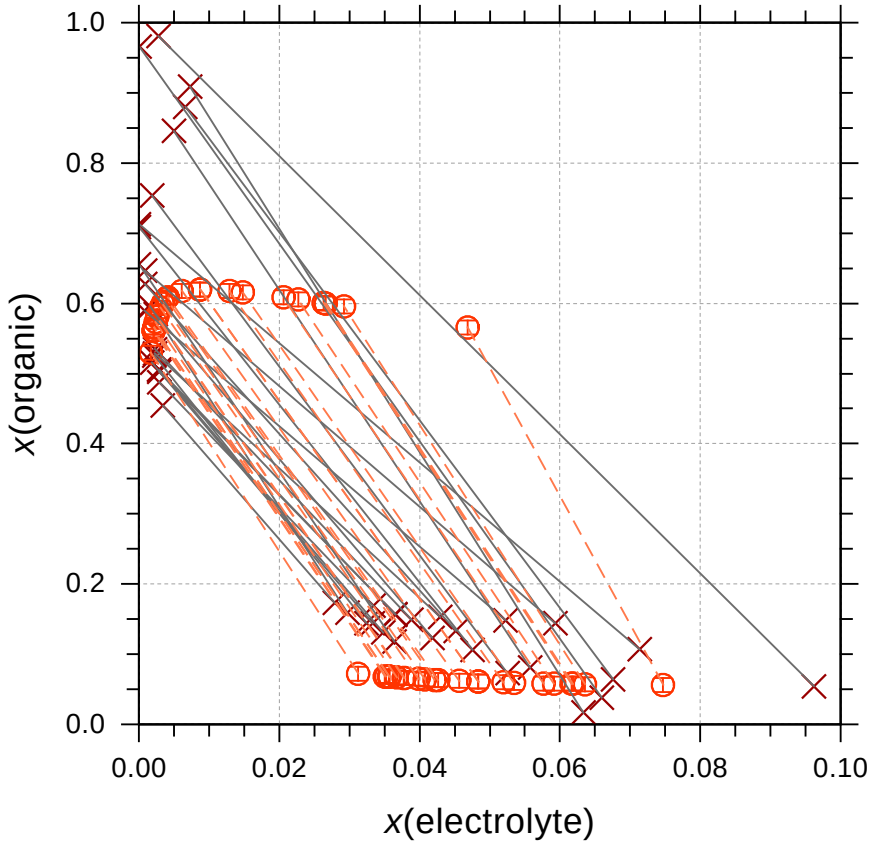
fval(1051) = 1.0046E+00

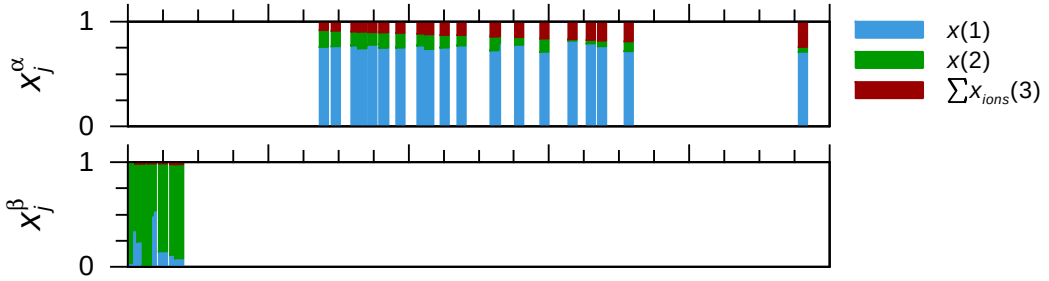
rel. contribution = 0.4777 %

Fig. S0285a (AIOMFAC_output_1051)

H_2O (1) + Acetone (2) + $CaCl_2$ (3)

Temperature: 296 K





left y-axis:

× CaCl2+Acetone+Water_LLE_Bourayou_2

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1051) = 1.000

dataset contribution to F_{obj}:

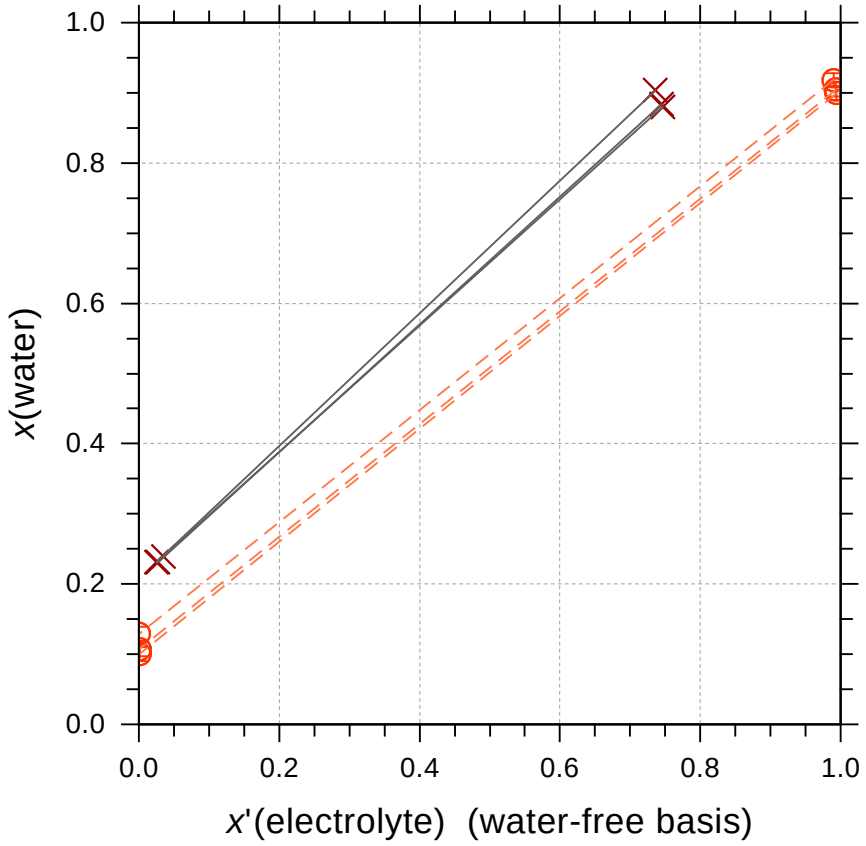
fval(1051) = 1.0046E+00

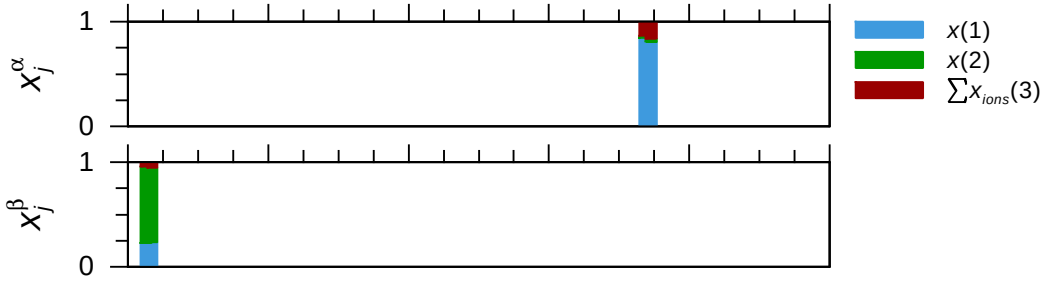
rel. contribution = 0.4777 %

Fig. S0286 (AIOMFAC_output_1022)

H_2O (1) + 3-Methyl-2-butanone (2) + HCl (3)

Temperature: 298 K





left y-axis:

× HCl+3-Methyl-2-butanone+Water_LLE_Pilloton

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(1022) = 0.050

dataset contribution to F_{obj}:

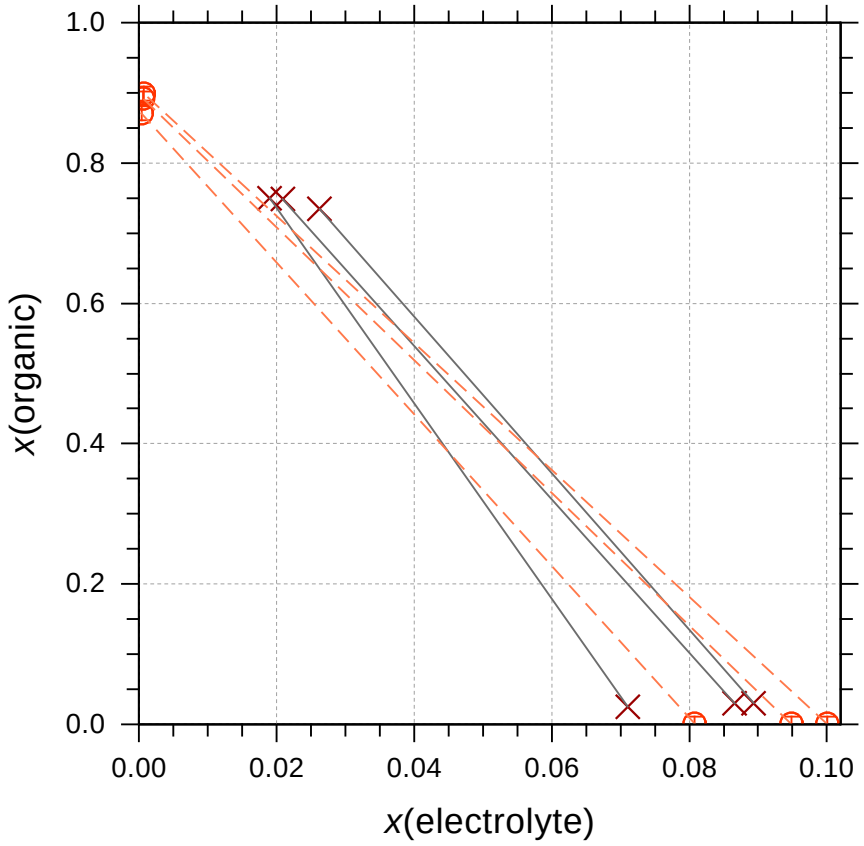
fval(1022) = 1.6213E+00

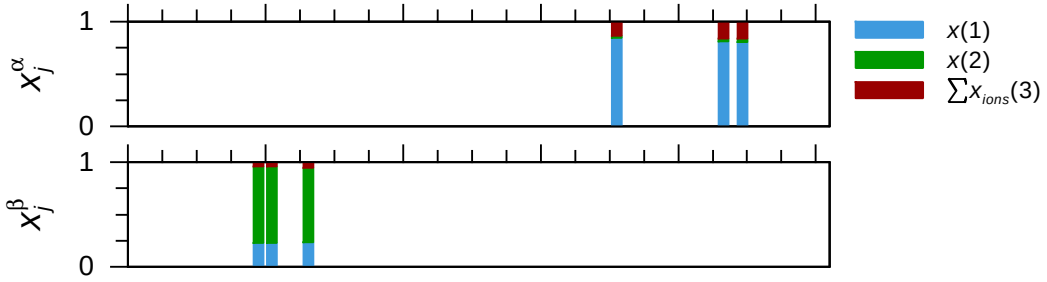
rel. contribution = 0.7710 %

Fig. S0286a (AIOMFAC_output_1022)

H_2O (1) + 3-Methyl-2-butanone (2) + HCl (3)

Temperature: 298 K





left y-axis:

× HCl+3-Methyl-2-butanone+Water_LLE_Pilloton

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(1022)$ = 0.050

dataset contribution to F_{obj}:

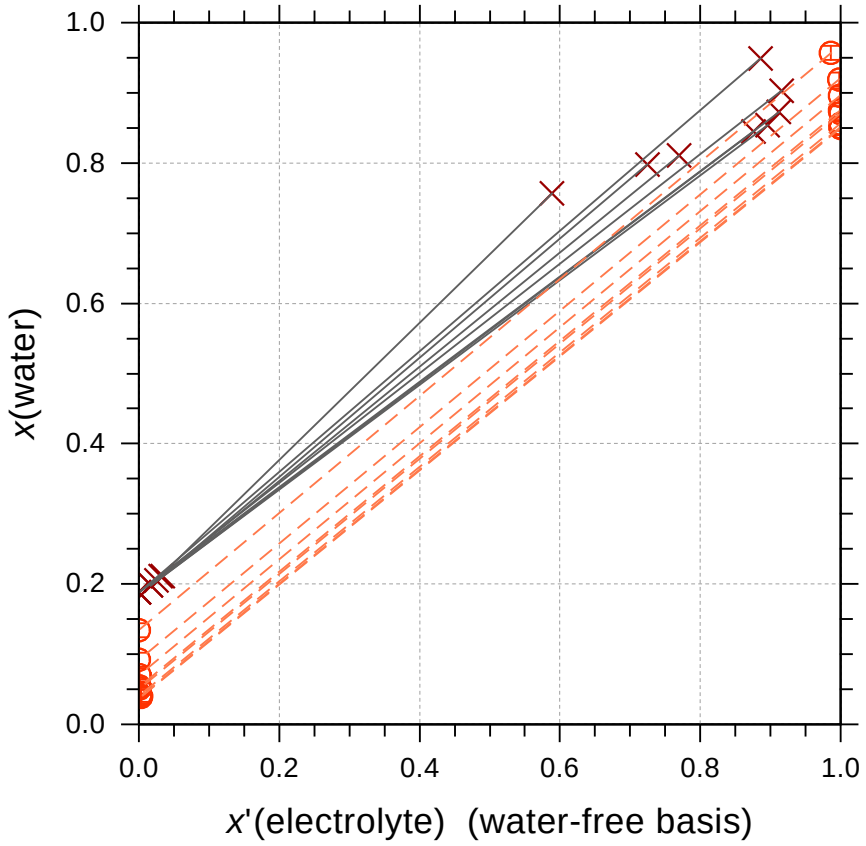
fval(1022) = 1.6213E+00

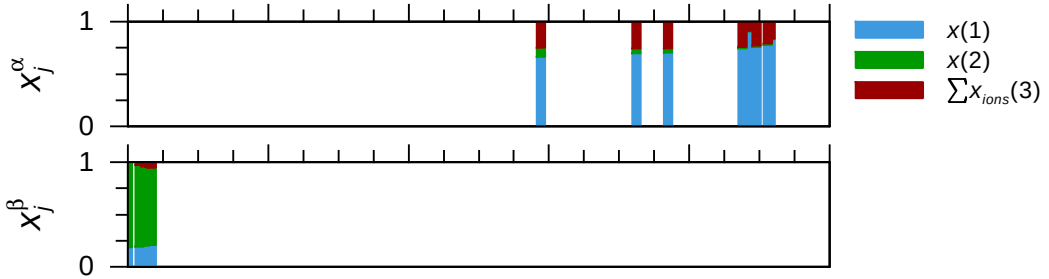
rel. contribution = 0.7710 %

Fig. S0287 (AIOMFAC_output_1023)

H_2O (1) + 4-Methyl-2-pentanone (2) + HCl (3)

Temperature: 298 K





left y-axis:

× HCl+4-Methyl-2-pentanone+Water_LLE_Pilloton

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(1023)$ = 0.050

dataset contribution to F_{obj}:

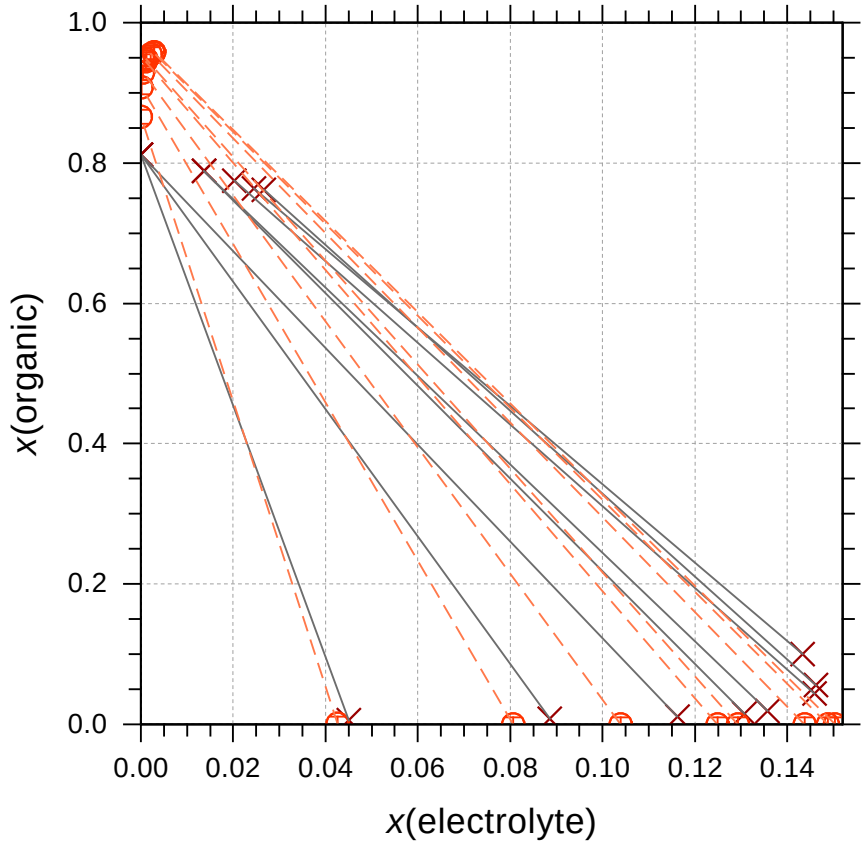
fval(1023) = 1.7983E+00

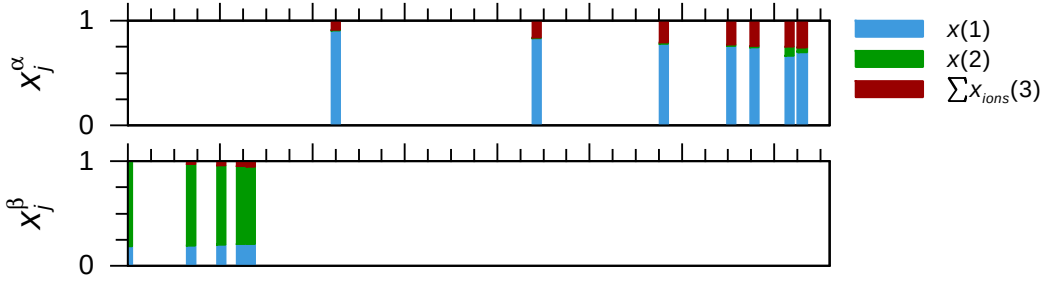
rel. contribution = 0.8551 %

Fig. S0287a (AIOMFAC_output_1023)

H_2O (1) + 4-Methyl-2-pentanone (2) + HCl (3)

Temperature: 298 K



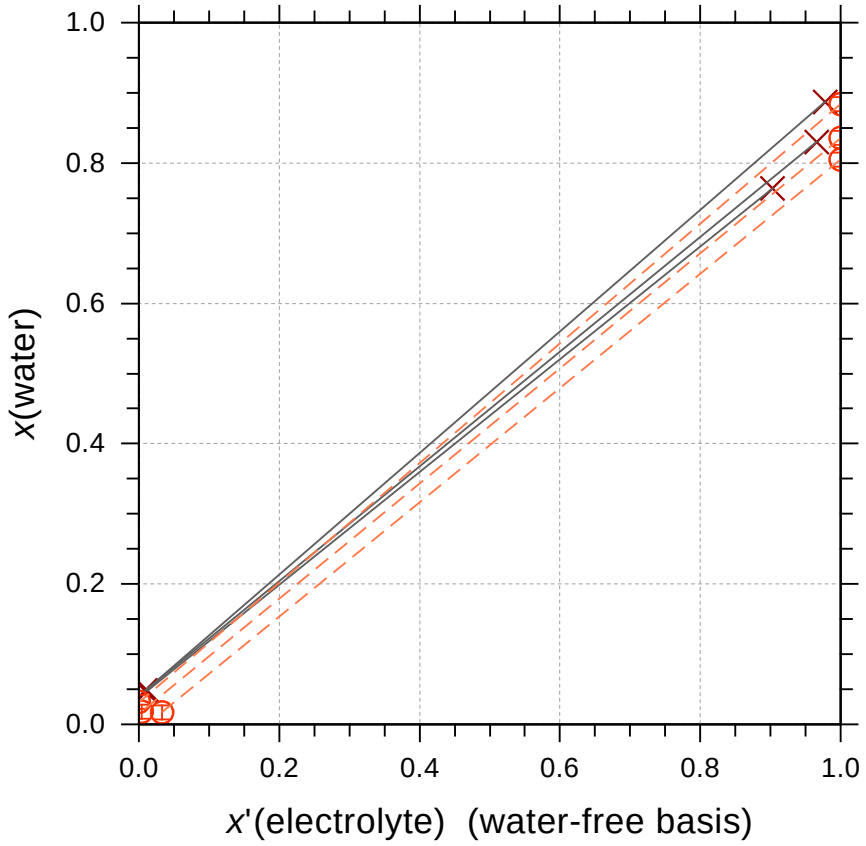


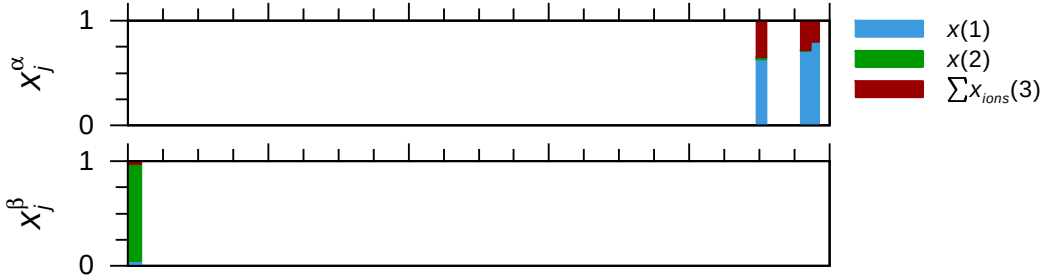
initial weighting of dataset:
$w^{init}(1023)$ = 0.050
dataset contribution to F_{obj}:
fval(1023) = 1.7983E+00
rel. contribution = 0.8551 %

Fig. S0288 (AIOMFAC_output_1024)

H_2O (1) + 3-Heptanone (2) + HCl (3)

Temperature: 298 K





left y-axis:

× HCl+3-Heptanone+Water_LLE_Pilloton

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(1024)$ = 0.050

dataset contribution to F_{obj}:

fval(1024) = 4.8833E-01

rel. contribution = 0.2322 %

Fig. S0288a (AIOMFAC_output_1024)

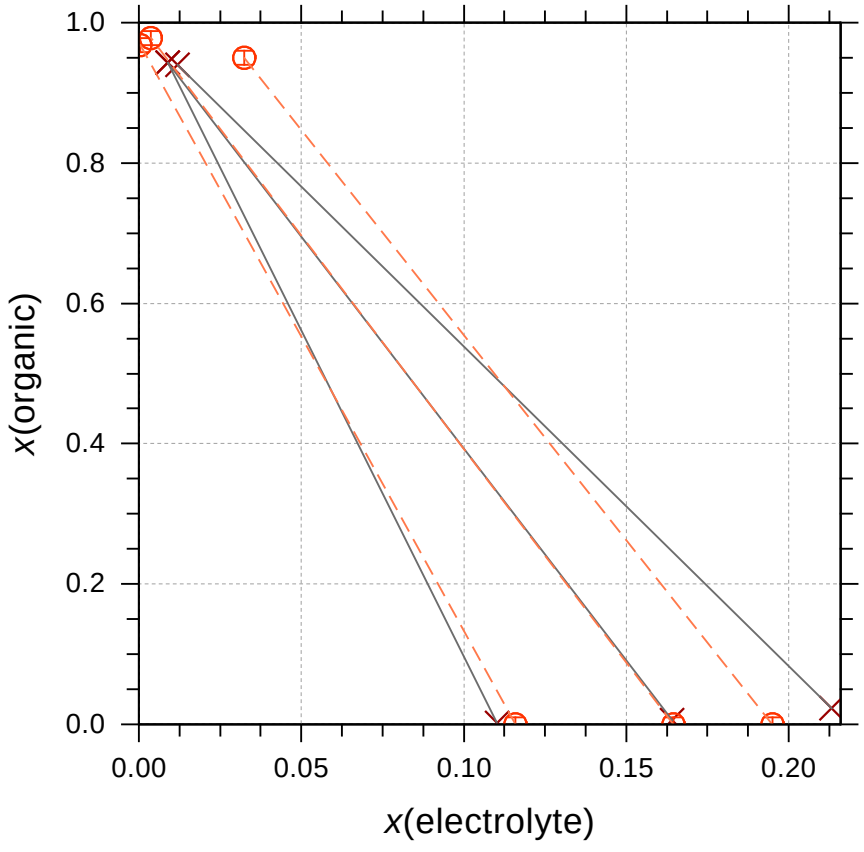
H_2O (1) + 3-Heptanone (2) + HCl (3)

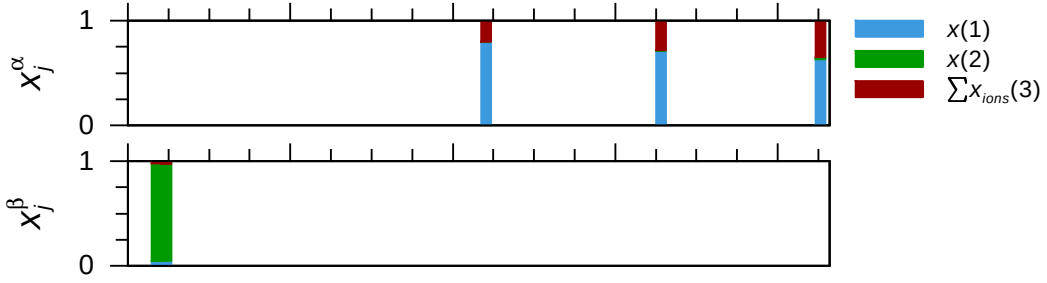
Temperature: 298 K

left y-axis:

× HCl+3-Heptanone+Water_LLE_Pilloton

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(1024)$ = 0.050

dataset contribution to F_{obj}:

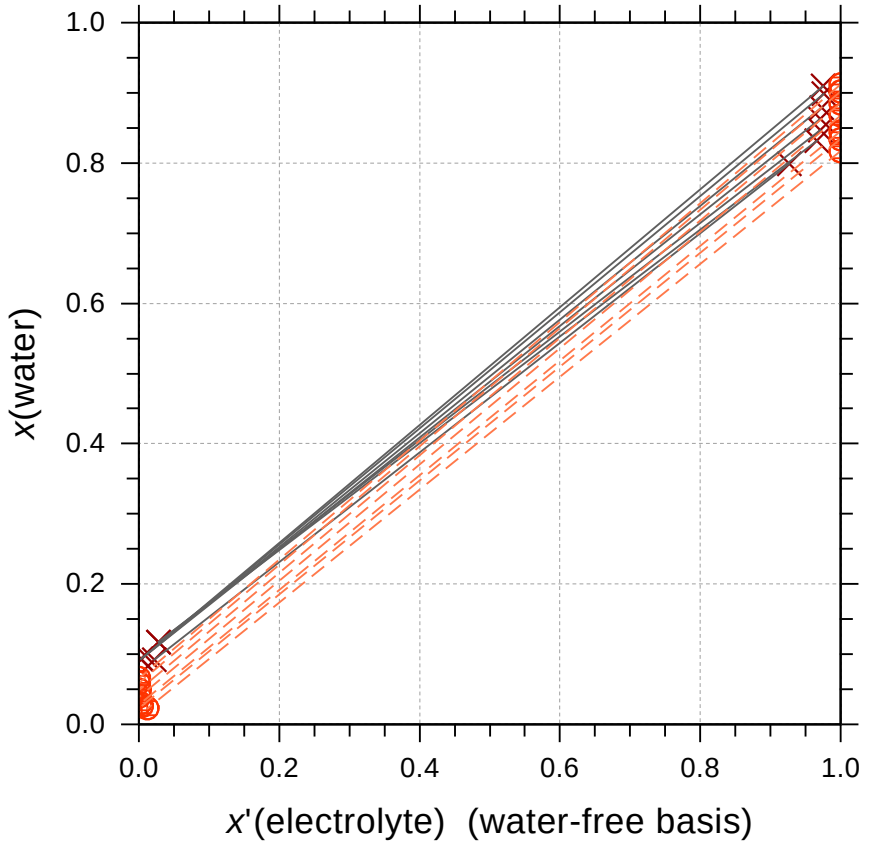
fval(1024) = 4.8833E-01

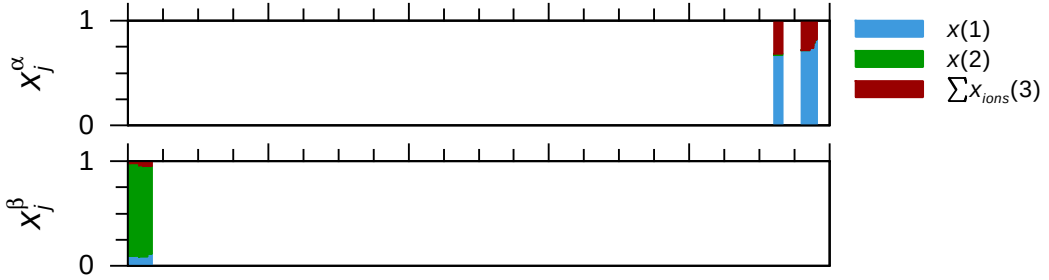
rel. contribution = 0.2322 %

Fig. S0289 (AIOMFAC_output_1025)

H_2O (1) + 2-Heptanone (2) + HCl (3)

Temperature: 298 K





left y-axis:

× HCl+2-Heptanone+Water_LLE_Pilloton

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(1025)$ = 0.050

dataset contribution to F_{obj}:

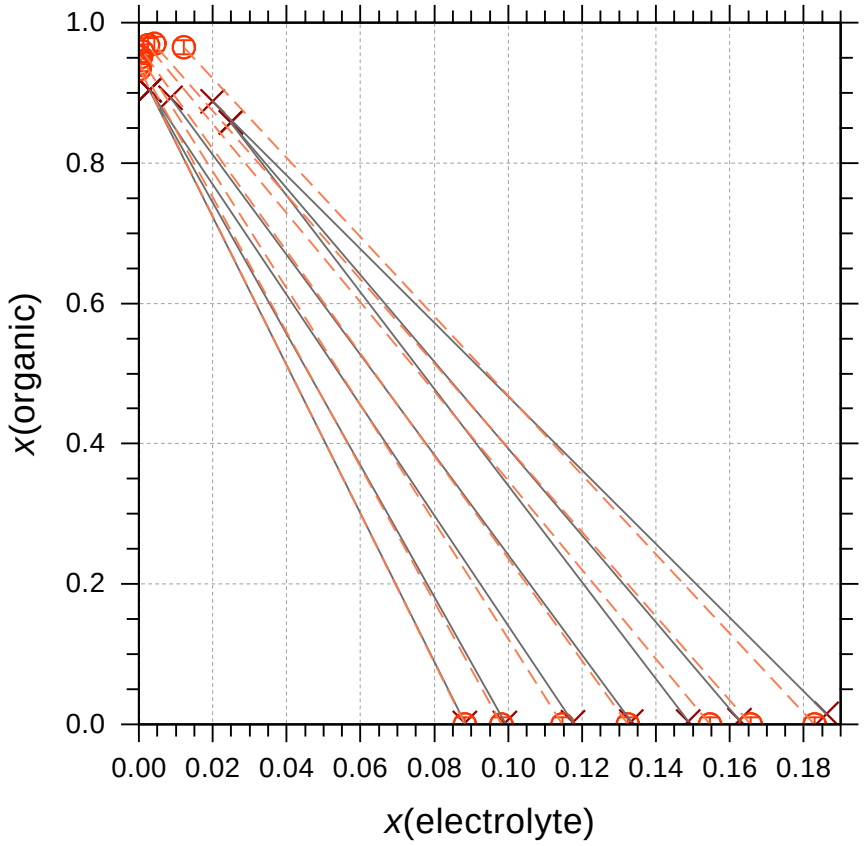
fval(1025) = 4.6413E-01

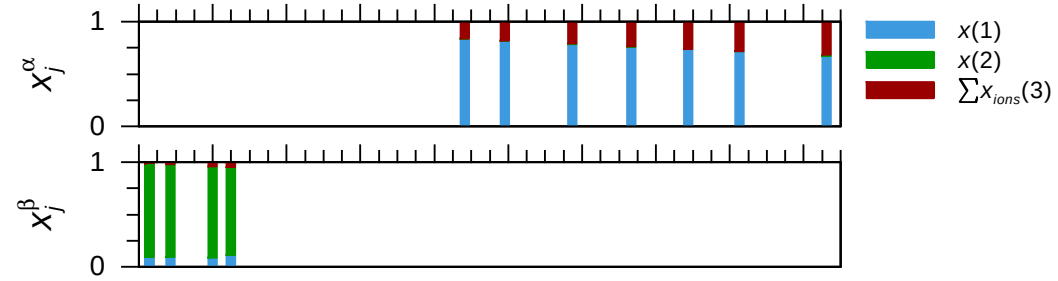
rel. contribution = 0.2207 %

Fig. S0289a (AIOMFAC_output_1025)

H_2O (1) + 2-Heptanone (2) + HCl (3)

Temperature: 298 K





left y-axis:

× HCl+2-Heptanone+Water_LLE_Pilloton

○ AIOMFAC calc. LLE composition

initial weighting of dataset:
$w^{init}(1025)$ = 0.050
dataset contribution to F_{obj}:
fval(1025) = 4.6413E-01
rel. contribution = 0.2207 %

Fig. S0290 (AIOMFAC_output_0326)

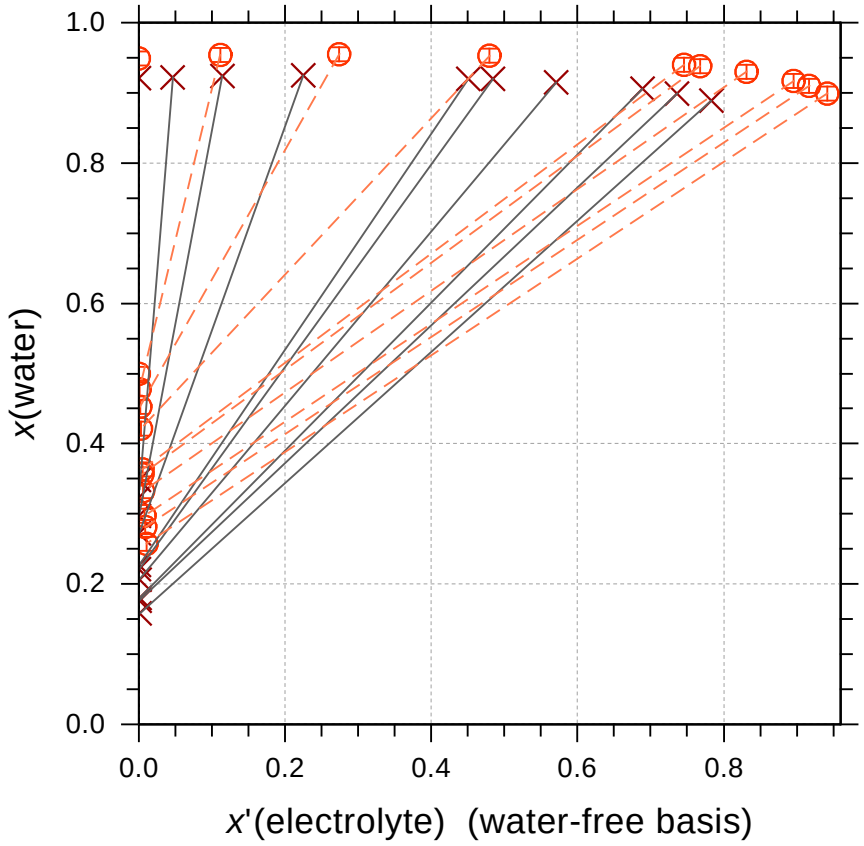
H_2O (1) + 2-Butanone (2) + KBr (3)

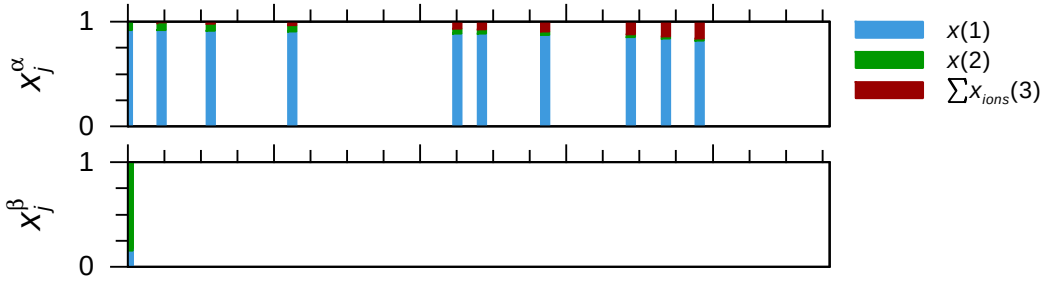
Temperature: 298 K

left y-axis:

× KBr+Butanone+Water_LLE_Li

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0326)$ = 1.000

dataset contribution to F_{obj}:

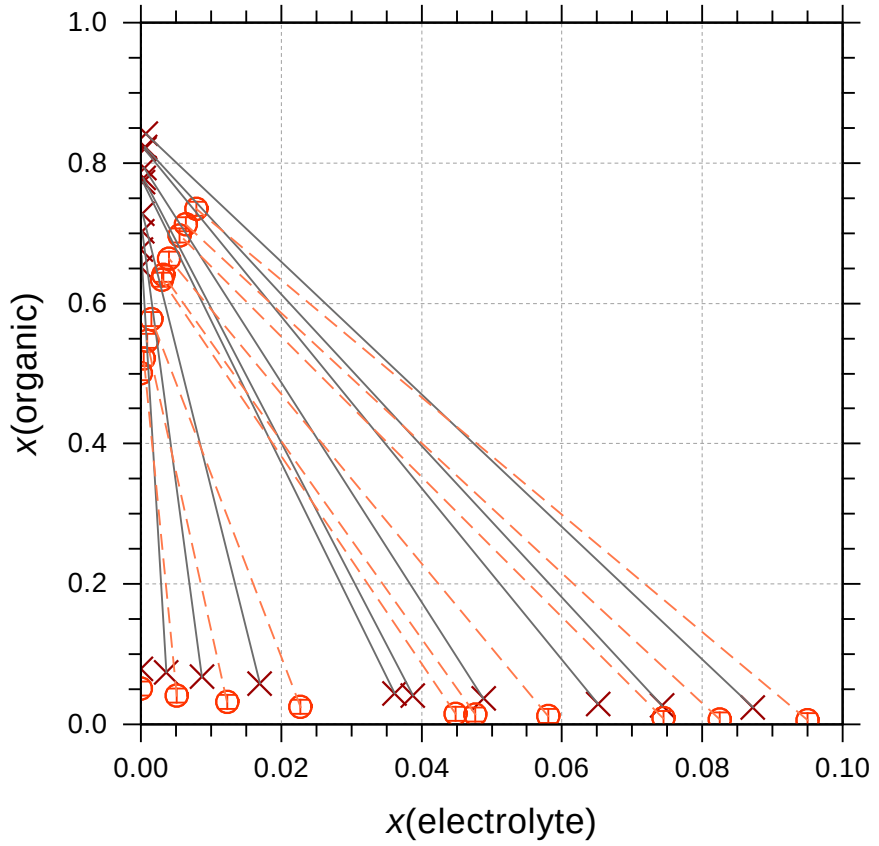
fval(0326) = 1.0395E+00

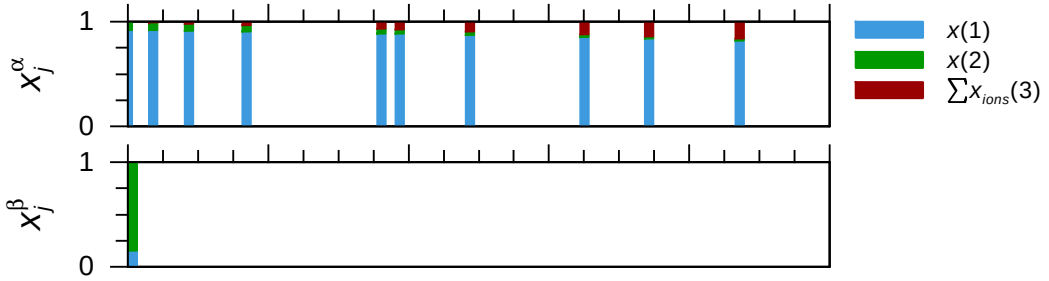
rel. contribution = 0.4943 %

Fig. S0290a (AIOMFAC_output_0326)

H_2O (1) + 2-Butanone (2) + KBr (3)

Temperature: 298 K



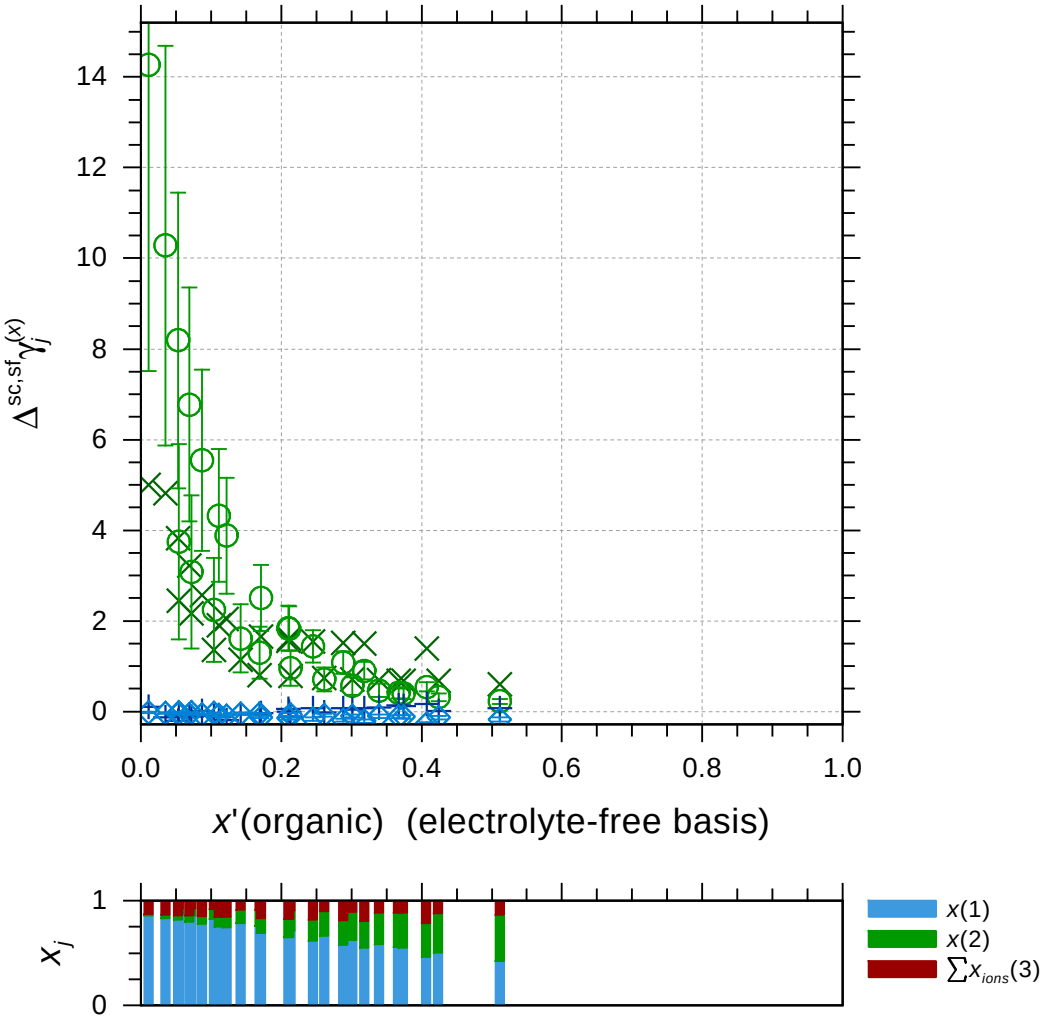


initial weighting of dataset:
$w^{init}(0326)$ = 1.000
dataset contribution to F_{obj}:
fval(0326) = 1.0395E+00
rel. contribution = 0.4943 %

Fig. S0291 (AIOMFAC_output_0359)

H_2O (1) + Acetone (2) + KBr (3)

Temperature range: 326 -- 363 K

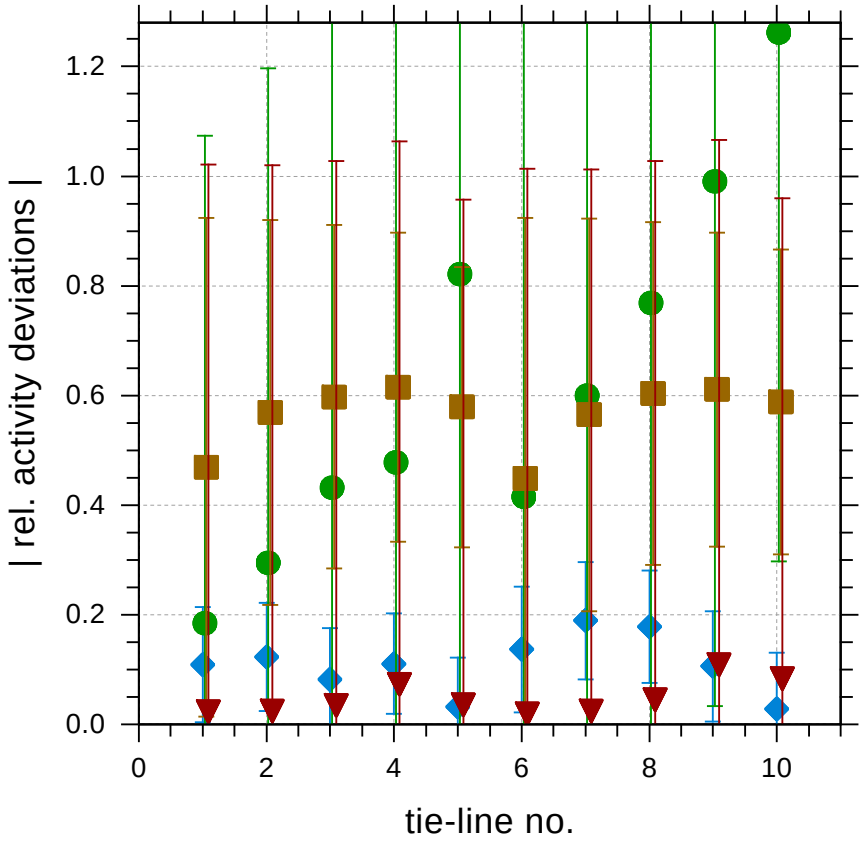


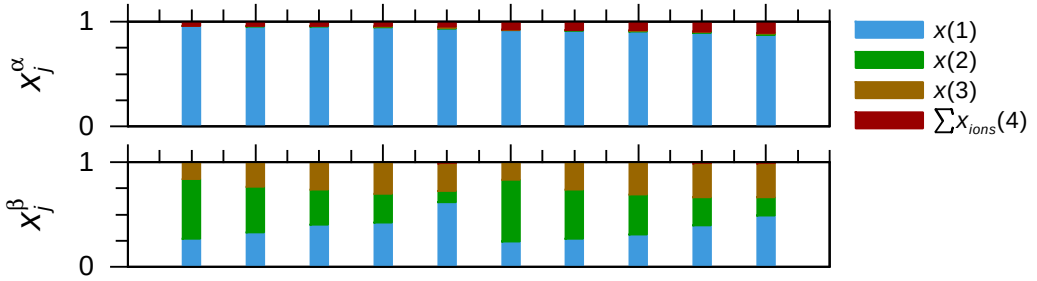
initial weighting of dataset:
$w^{init}(0359)$ = 0.500
dataset contribution to F_{obj}:
fval(0359) = 6.3918E-01
rel. contribution = 0.3040 %

Fig. S0292 (AIOMFAC_output_0318)

H_2O (1) + 4-Methyl-2-pentanone (2) + Propanoic_acid (3) + KCl (4)

Temperature: 298 K





left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

initial weighting of dataset:
w^{init}(0318) = 1.000
dataset contribution to F_{obj}:
fval(0318) = 4.1500E+00
rel. contribution = 1.9735 %

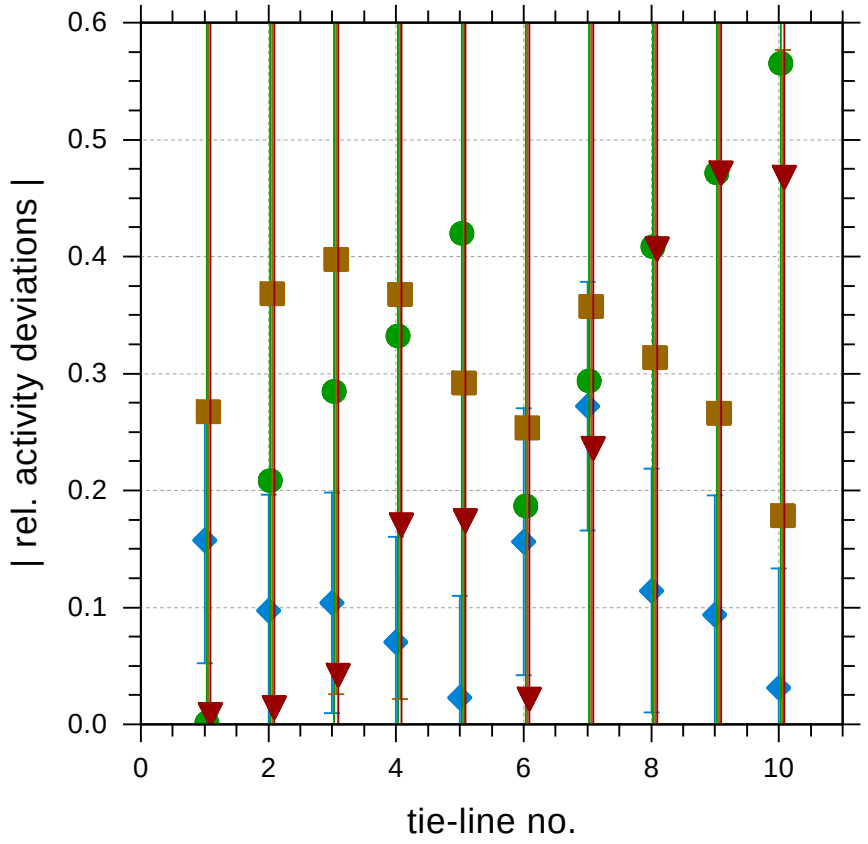
Fig. S0293 (AIOMFAC_output_0320)

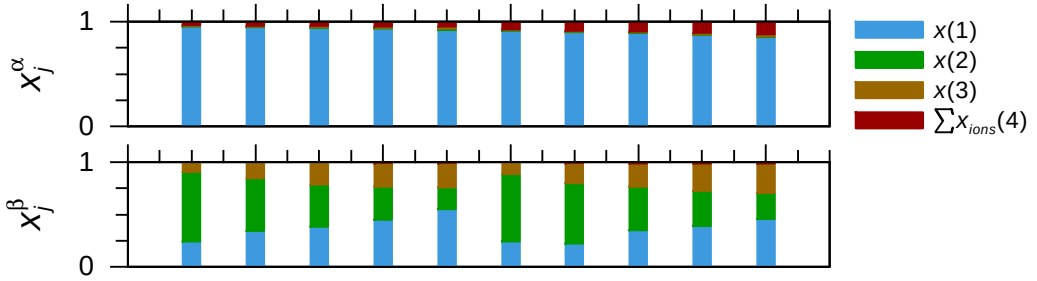
H_2O (1) + 3-Methyl-2-butanone (2) + Propanoic_acid (3) + KCl (4)

Temperature: 298 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



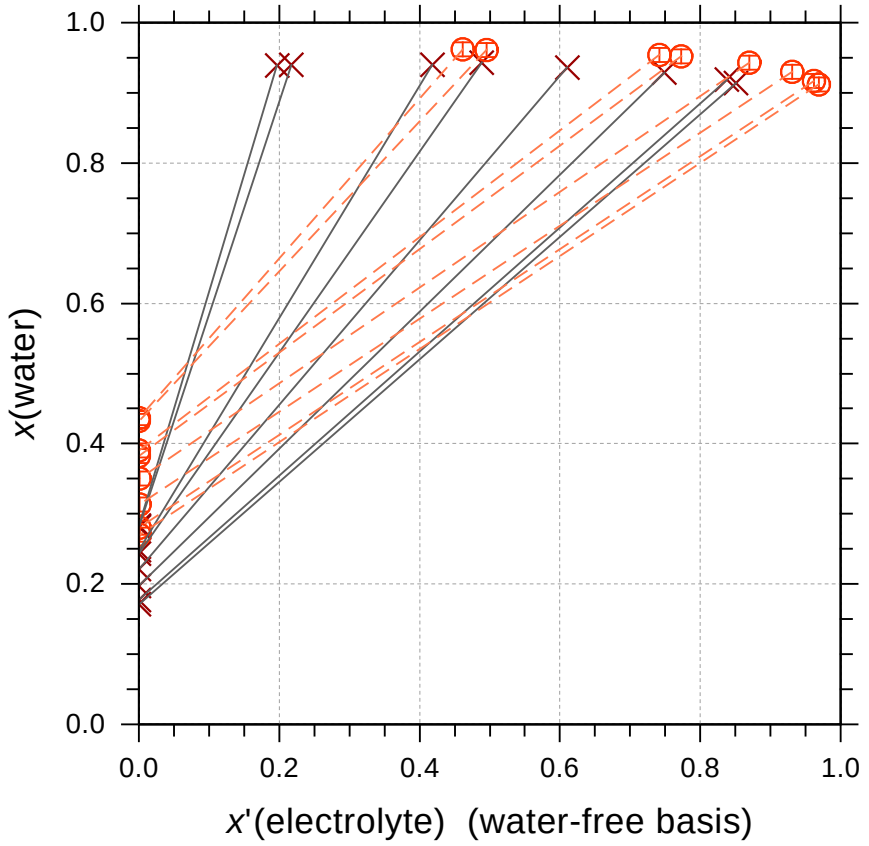


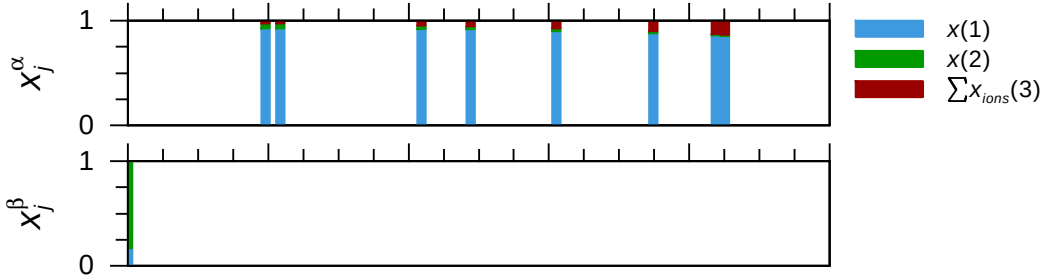
initial weighting of dataset:
$w^{init}(0320)$ = 1.000
dataset contribution to F_{obj}:
fval(0320) = 1.5576E+00
rel. contribution = 0.7407 %

Fig. S0294 (AIOMFAC_output_0322)

H_2O (1) + 2-Butanone (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl+Butanone+Water_LLE_Tan

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0322) = 1.000

dataset contribution to F_{obj}:

fval(0322) = 7.1812E-01

rel. contribution = 0.3415 %

Fig. S0294a (AIOMFAC_output_0322)

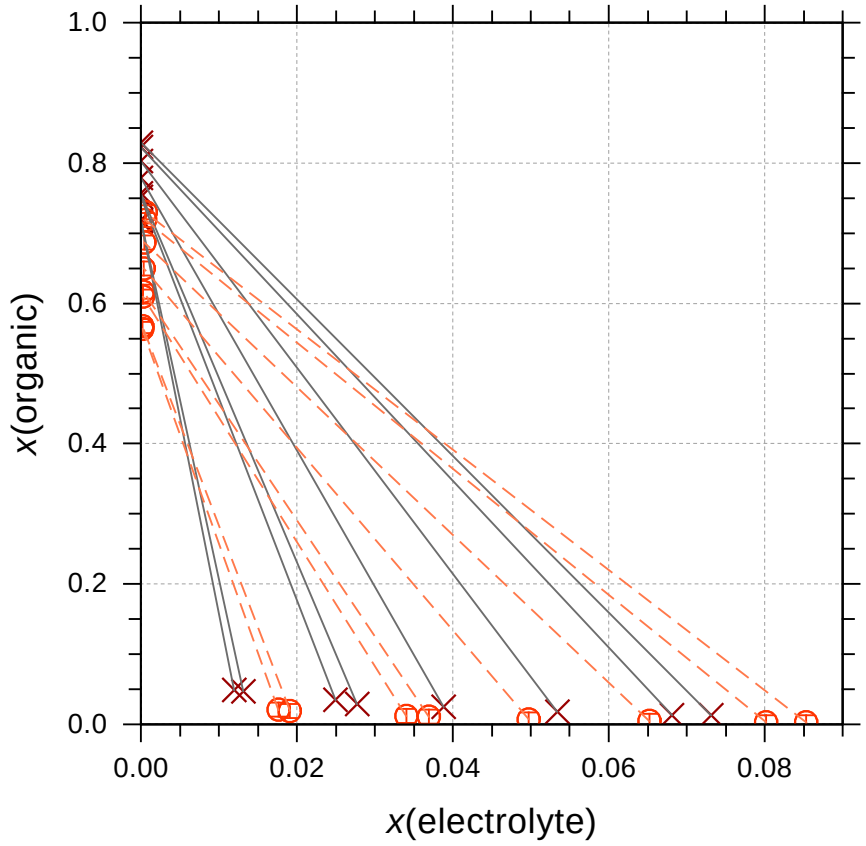
H_2O (1) + 2-Butanone (2) + KCl (3)

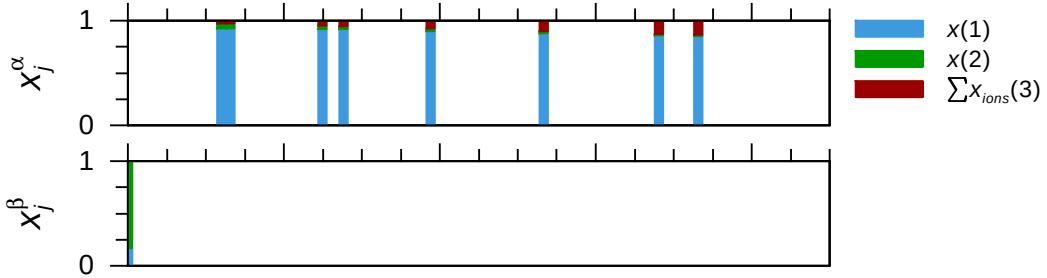
Temperature: 298 K

left y-axis:

× KCl+Butanone+Water_LLE_Tan

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0322)$ = 1.000

dataset contribution to F_{obj}:

fval(0322) = 7.1812E-01

rel. contribution = 0.3415 %

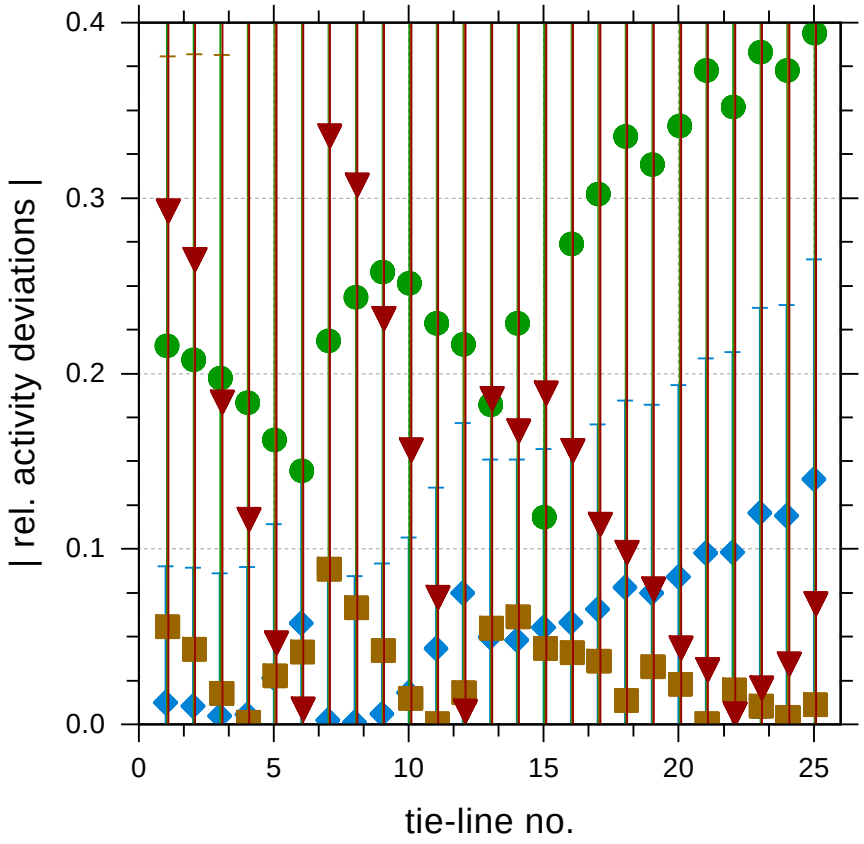
Fig. S0295 (AIOMFAC_output_0323)

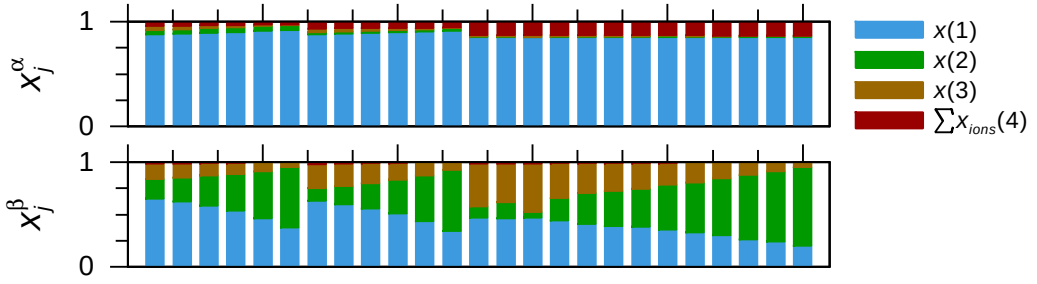
H_2O (1) + 2-Butanone (2) + 1-Propanol (3) + KCl (4)

Temperature: 298 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



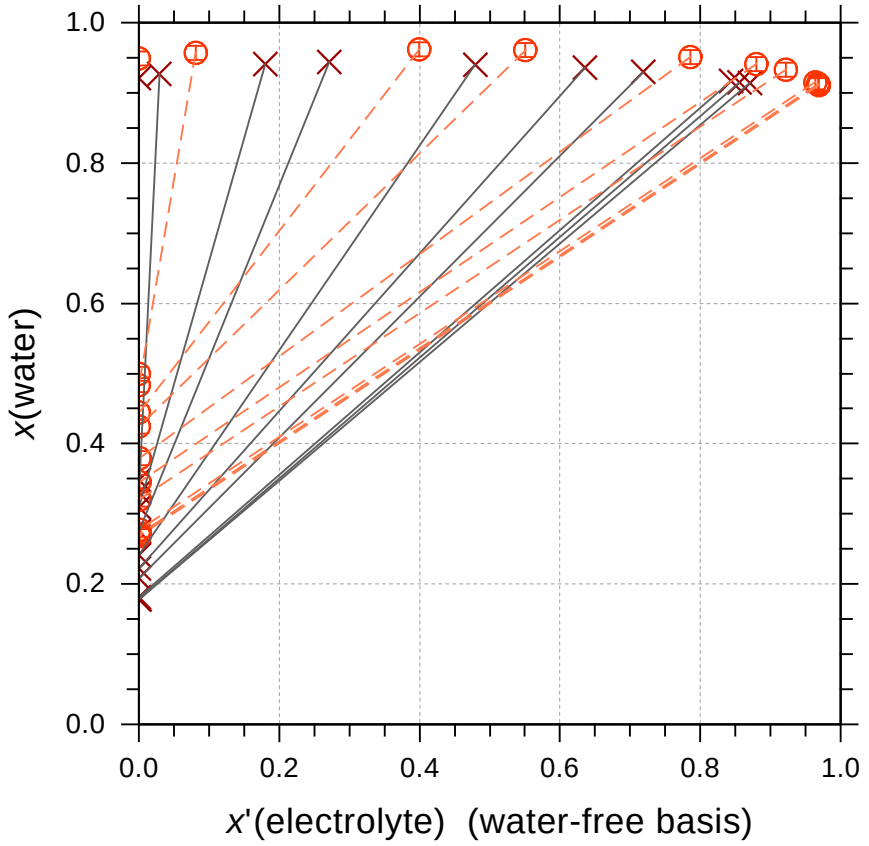


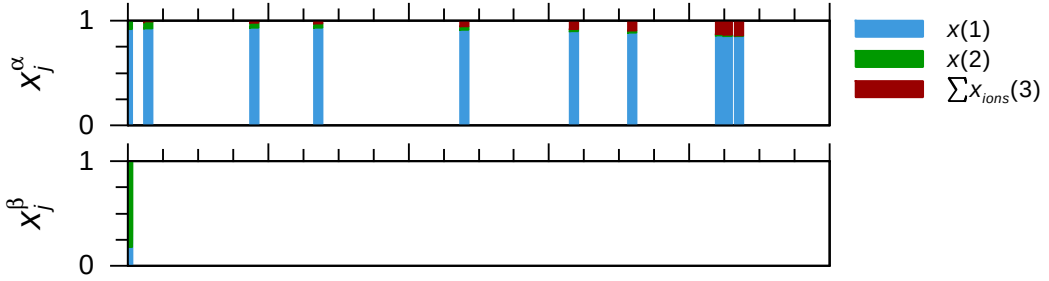
initial weighting of dataset:
$w^{init}(0323)$ = 1.000
dataset contribution to F_{obj}:
fval(0323) = 5.3040E-01
rel. contribution = 0.2522 %

Fig. S0296 (AIOMFAC_output_0324)

H_2O (1) + 2-Butanone (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl+Butanone+Water_LLE_Li

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0324) = 1.000

dataset contribution to F_{obj}:

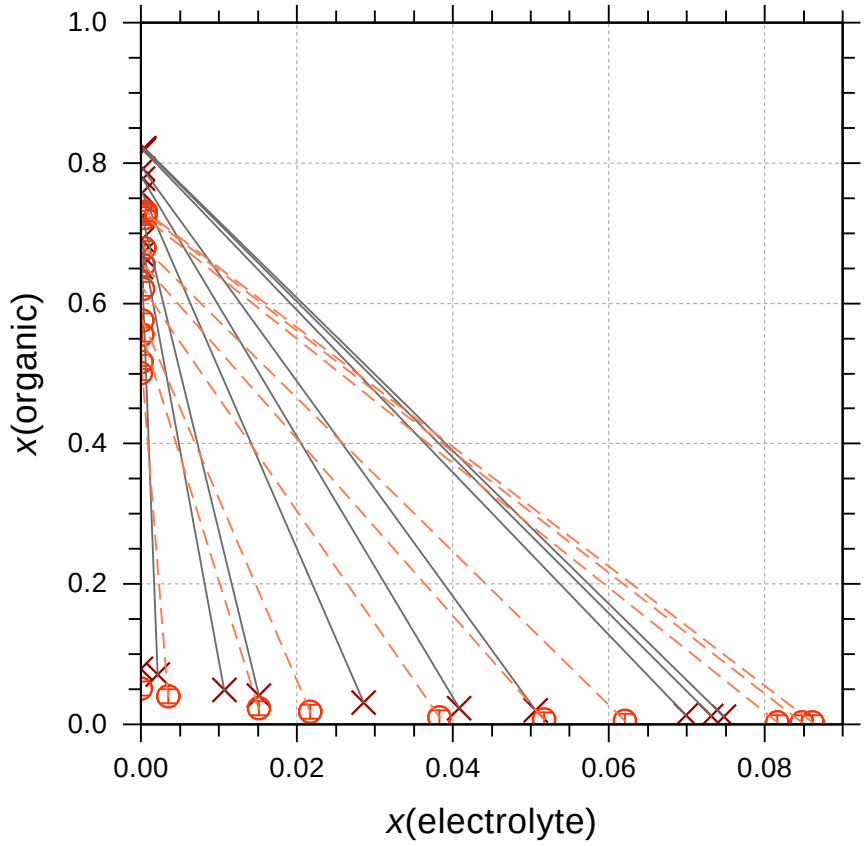
fval(0324) = 6.2662E-01

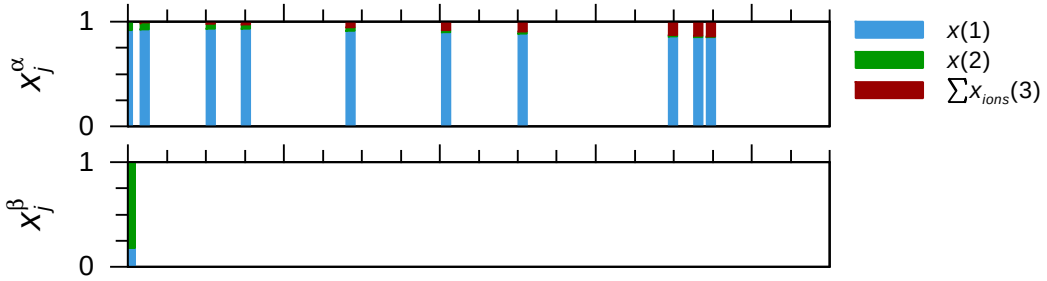
rel. contribution = 0.2980 %

Fig. S0296a (AIOMFAC_output_0324)

H_2O (1) + 2-Butanone (2) + KCl (3)

Temperature: 298 K



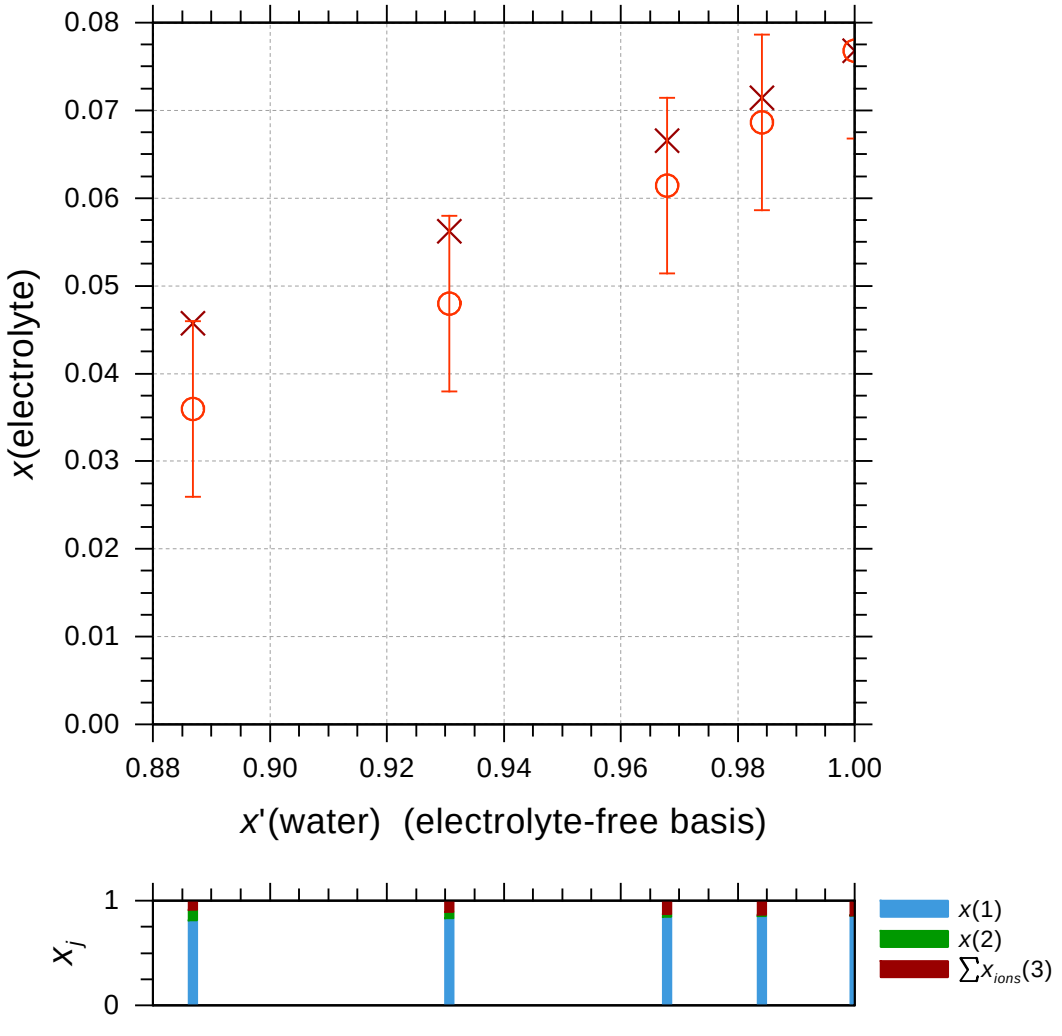


initial weighting of dataset:
w^{init}(0324) = 1.000
dataset contribution to F_{obj}:
fval(0324) = 6.2662E-01
rel. contribution = 0.2980 %

Fig. S0297 (AIOMFAC_output_0360)

H_2O (1) + Acetone (2) + KCl (3)

Temperature: 293 K

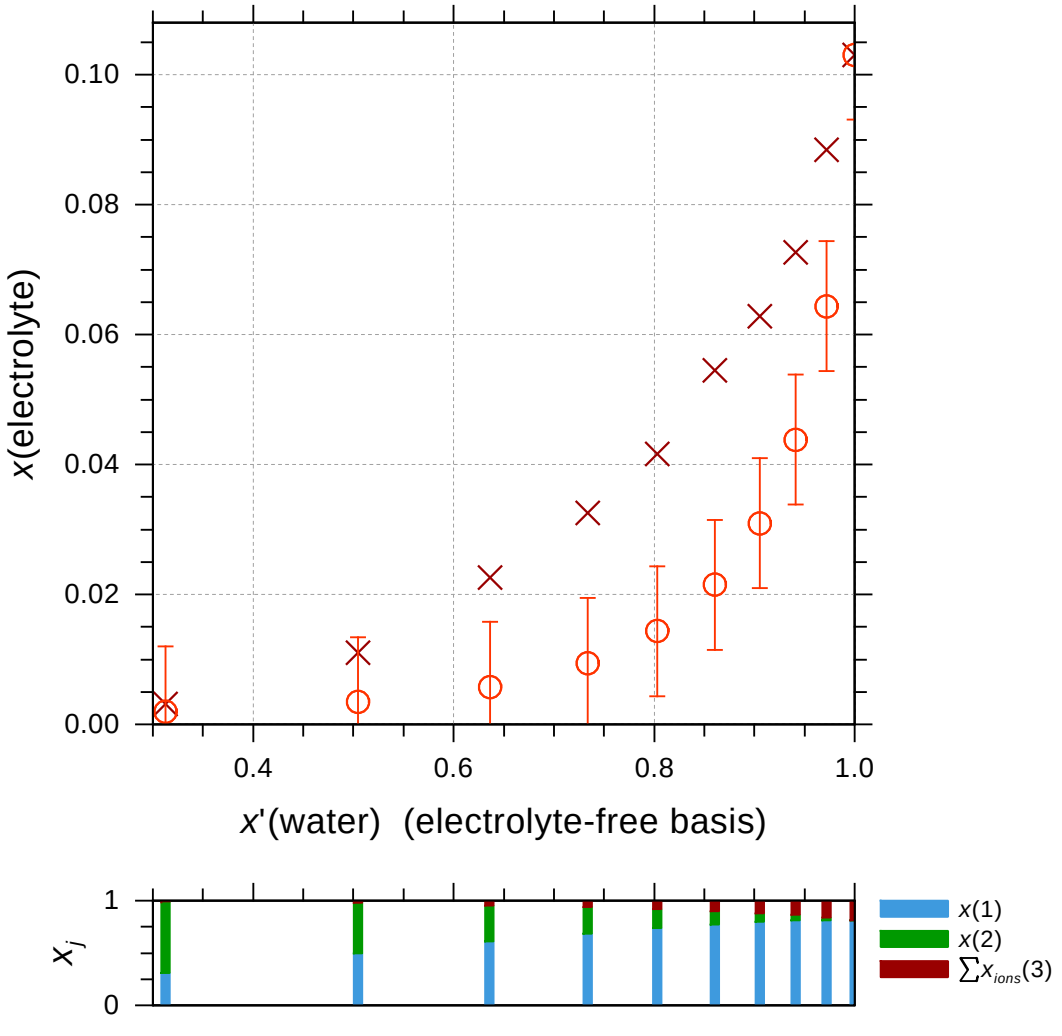


initial weighting of dataset:
$w^{init}(0360)$ = 0.800
dataset contribution to F_{obj}:
fval(0360) = 4.1714E-02
rel. contribution = 0.0198 %

Fig. S0298 (AIOMFAC_output_0943)

H_2O (1) + Acetone (2) + KNO_3 (3)

Temperature: 313 K

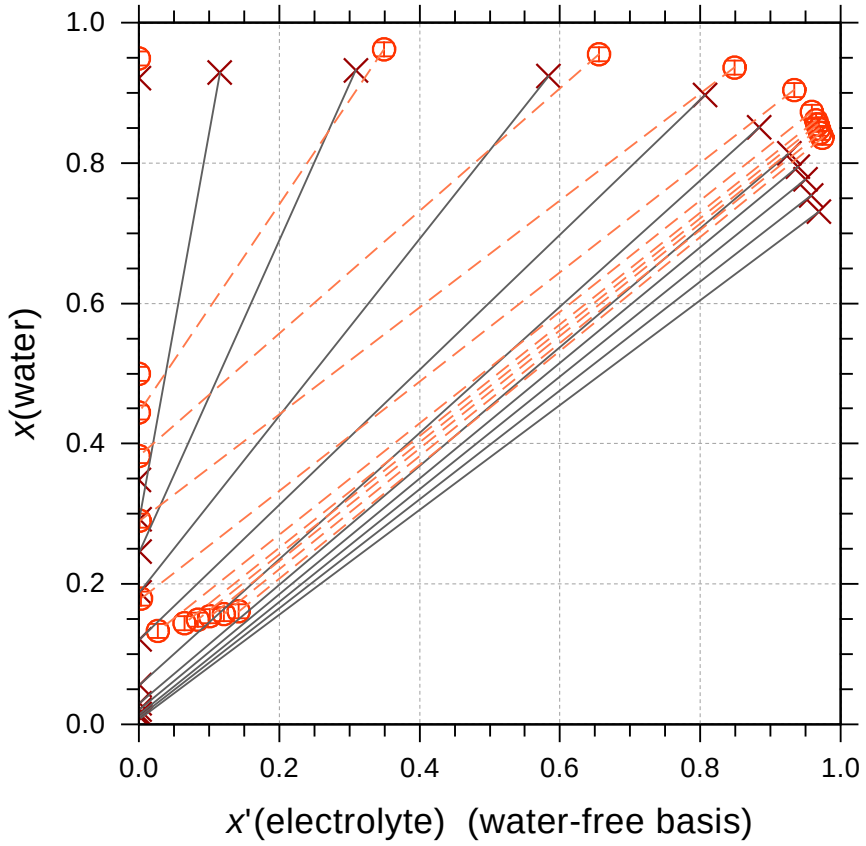


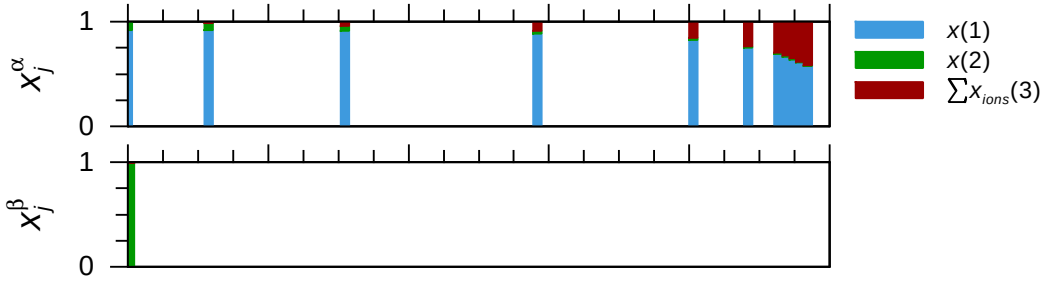
initial weighting of dataset:
$w^{init}(0943)$ = 0.600
dataset contribution to F_{obj}:
fval(0943) = 9.7507E-01
rel. contribution = 0.4637 %

Fig. S0299 (AIOMFAC_output_0345)

H_2O (1) + 2-Butanone (2) + LiCl (3)

Temperature: 298 K





left y-axis:

× LiCl+Butanone+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0345) = 1.000

dataset contribution to F_{obj}:

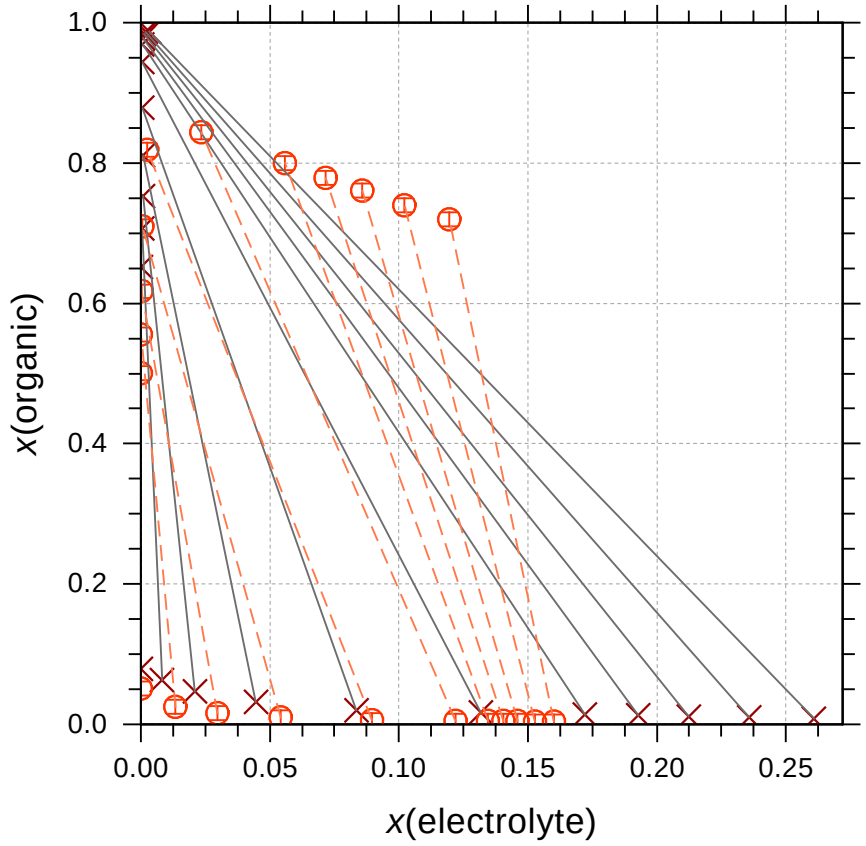
fval(0345) = 1.8225E+00

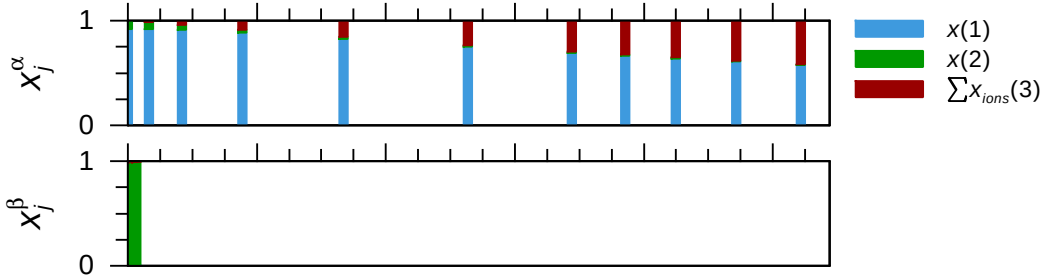
rel. contribution = 0.8667 %

Fig. S0299a (AIOMFAC_output_0345)

H_2O (1) + 2-Butanone (2) + LiCl (3)

Temperature: 298 K





left y-axis:

× LiCl+Butanone+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0345) = 1.000

dataset contribution to F_{obj}:

fval(0345) = 1.8225E+00

rel. contribution = 0.8667 %

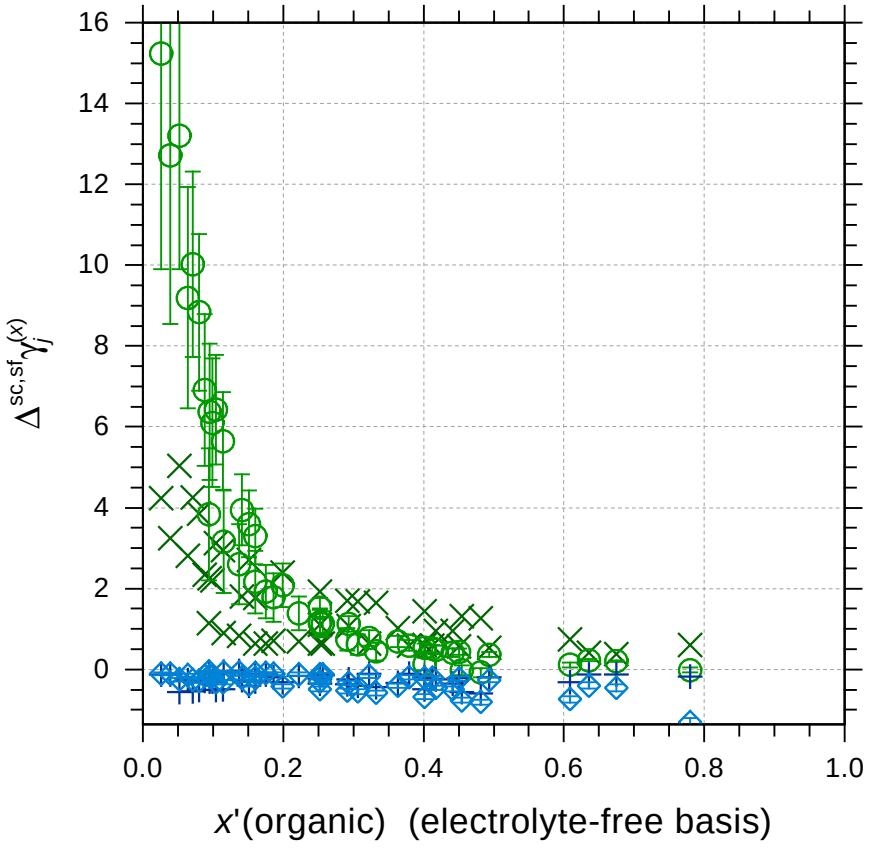
Fig. S0300 (AIOMFAC_output_0357)

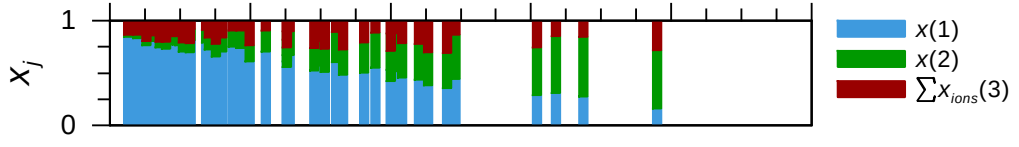
H_2O (1) + Acetone (2) + LiCl (3)

Temperature range: 329 -- 356 K

left y-axis:

- LiCl+Acetone+Water_VLE_Al-Sahhaf (EXP, org.)
- AIOMFAC $\Delta^{sc,sf}\gamma^{(x)}_{org.}$
- LiCl+Acetone+Water_VLE_Al-Sahhaf (EXP, water)
- AIOMFAC $\Delta^{sc,sf}\gamma^{(x)}_{w}$



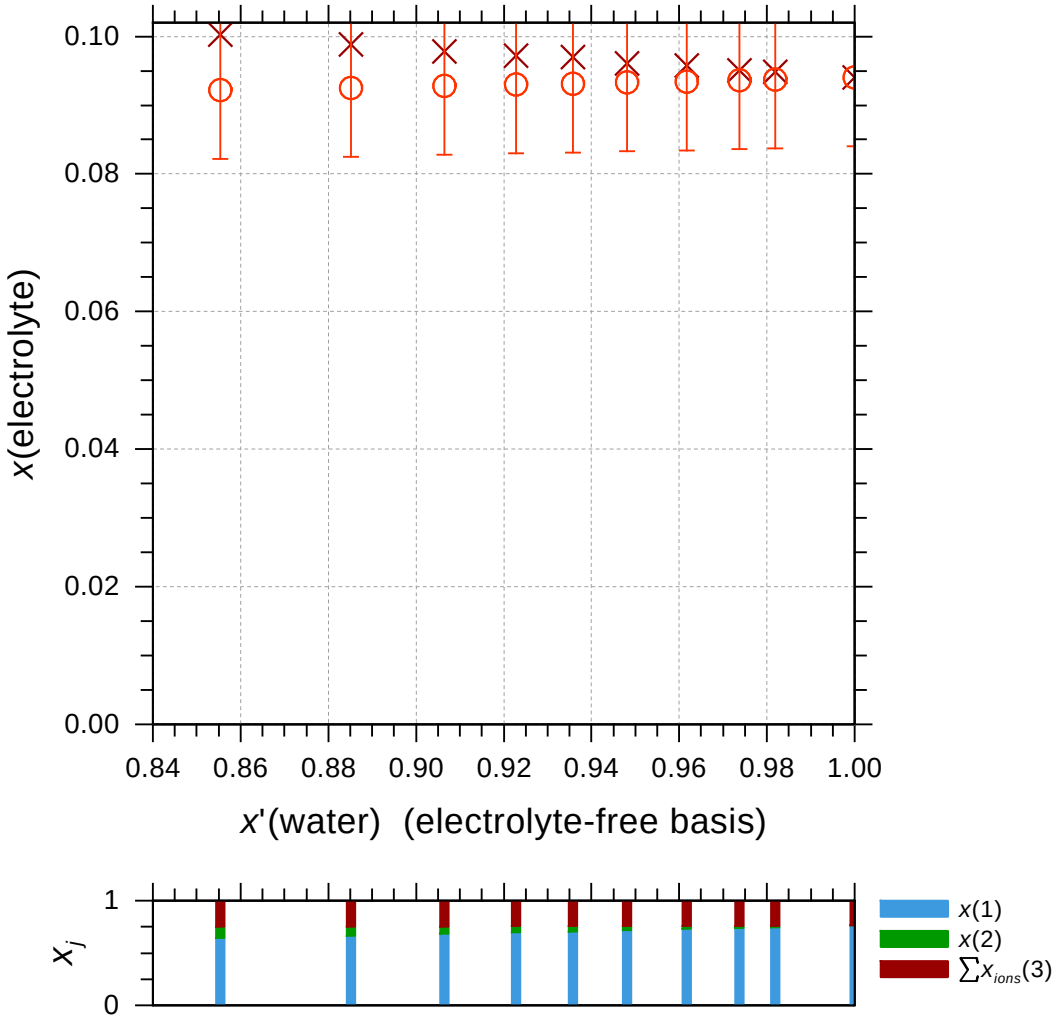


initial weighting of dataset:
$w^{init}(0357)$ = 0.500
dataset contribution to F_{obj}:
fval(0357) = 1.5541E+00
rel. contribution = 0.7390 %

Fig. S0301 (AIOMFAC_output_0361)

H_2O (1) + Acetone (2) + $MgCl_2$ (3)

Temperature: 293 K

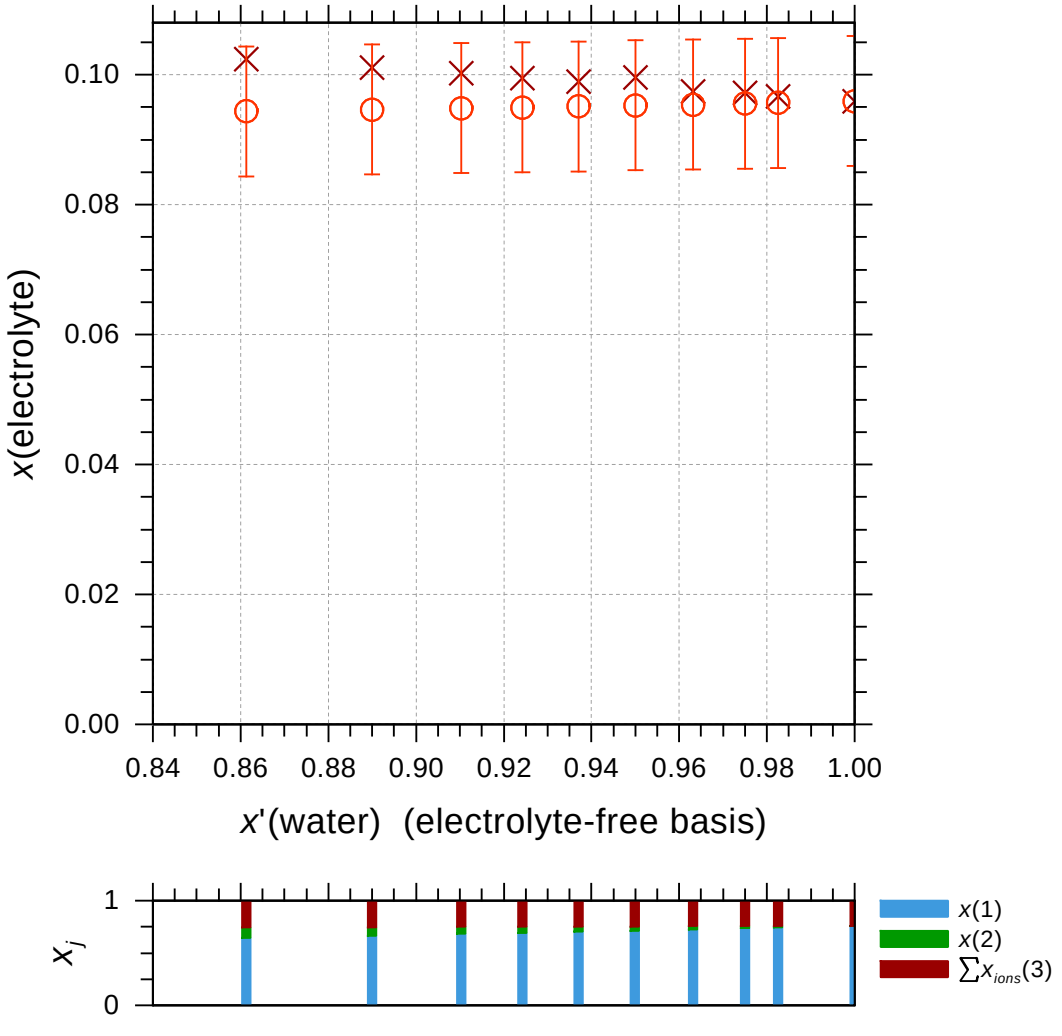


initial weighting of dataset:
$w^{init}(0361)$ = 0.800
dataset contribution to F_{obj}:
fval(0361) = 1.2509E-02
rel. contribution = 0.0059 %

Fig. S0302 (AIOMFAC_output_0362)

H_2O (1) + Acetone (2) + $MgCl_2$ (3)

Temperature: 303 K

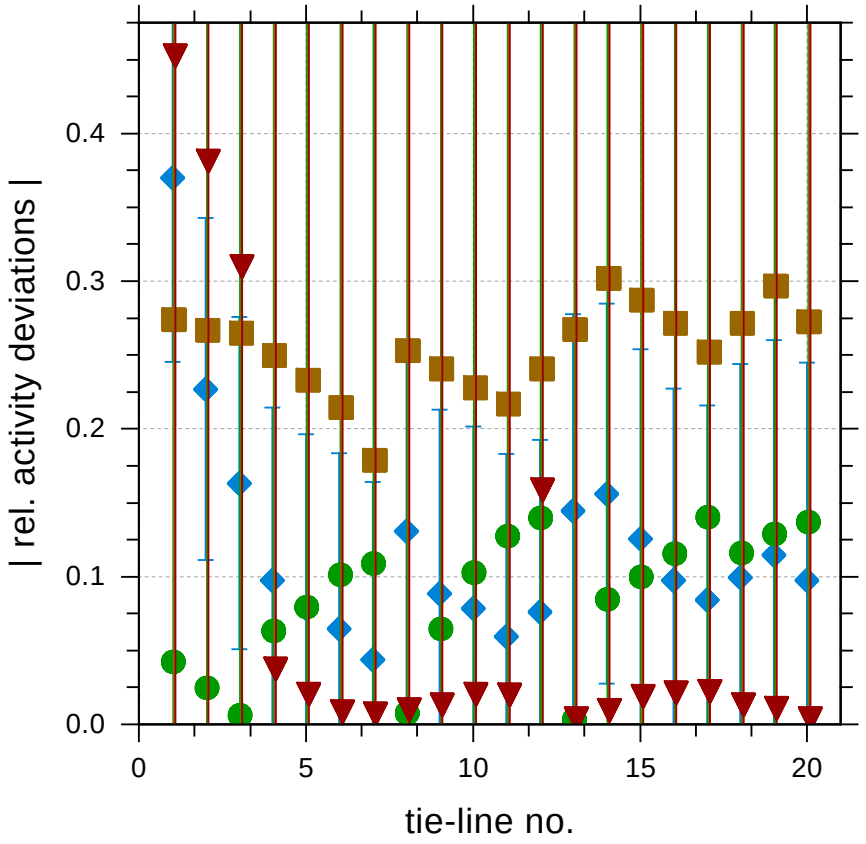


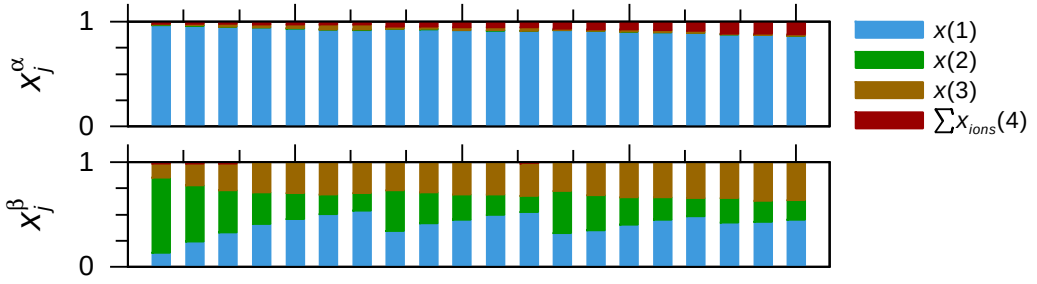
initial weighting of dataset:
w^{init}(0362) = 0.800
dataset contribution to F_{obj}:
fval(0362) = 1.3203E-02
rel. contribution = 0.0063 %

Fig. S0303 (AIOMFAC_output_0304)

H_2O (1) + 4-Methyl-2-pentanone (2) + Propanoic_acid (3) + Na_2SO_4 (4)

Temperature: 308 K





left y-axis:

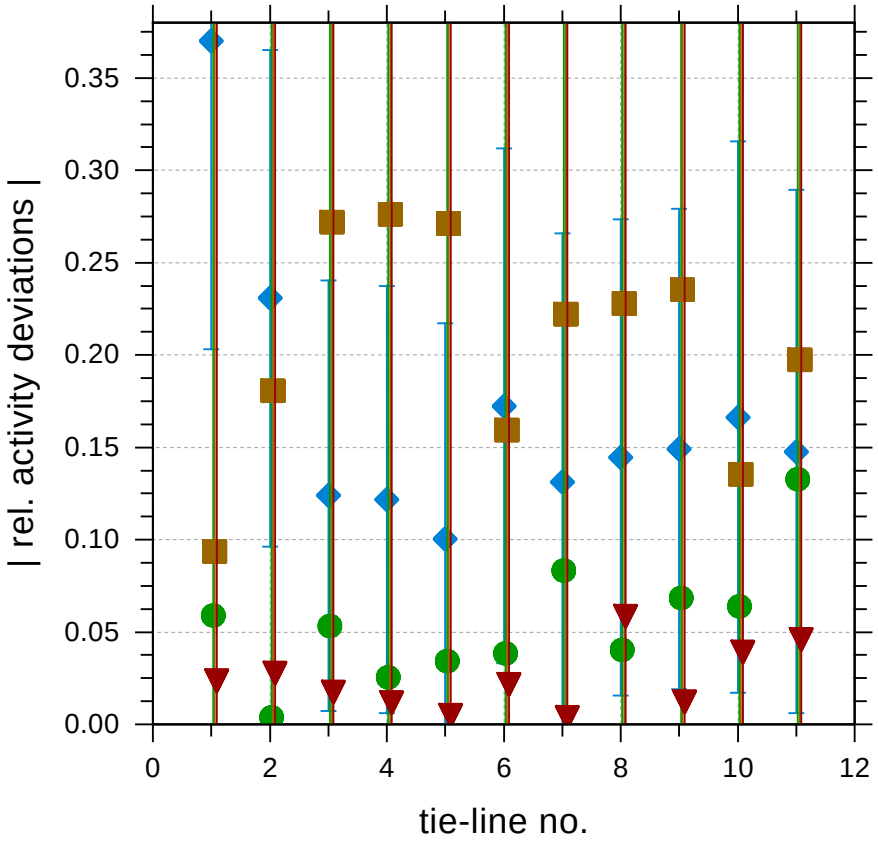
- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

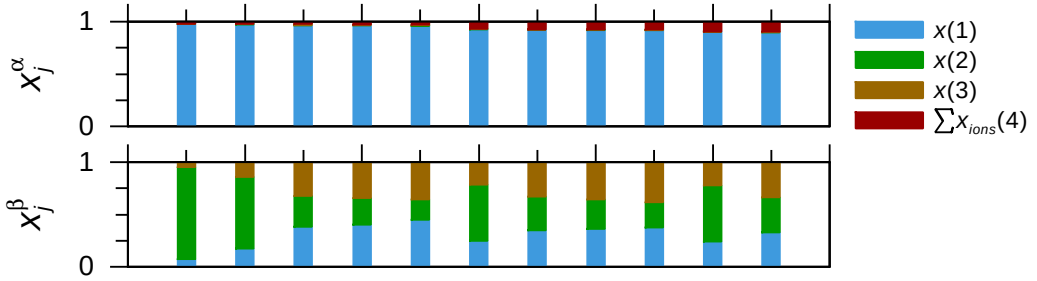
initial weighting of dataset:
$w^{init}(0304)$ = 1.000
dataset contribution to F_{obj}:
fval(0304) = 5.8900E-01
rel. contribution = 0.2801 %

Fig. S0304 (AIOMFAC_output_0308)

H_2O (1) + 4-Methyl-2-pentanone (2) + Butyric_acid (3) + Na_2SO_4 (4)

Temperature: 308 K





left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

initial weighting of dataset:
w^{init}(0308) = 1.000
dataset contribution to F_{obj}:
fval(0308) = 4.2202E-01
rel. contribution = 0.2007 %

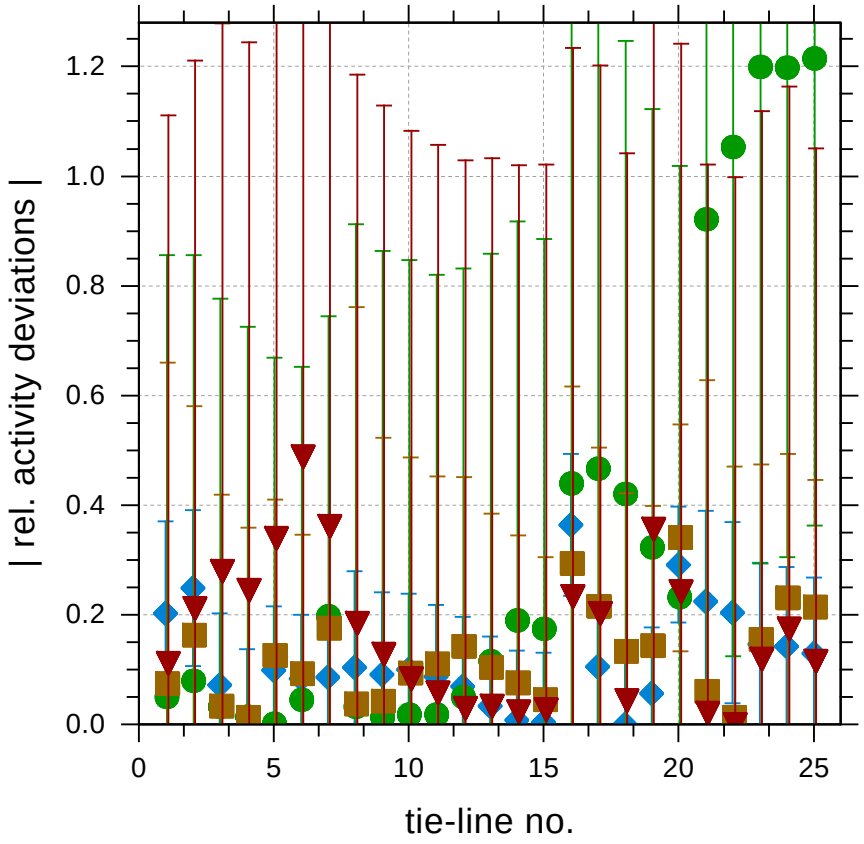
Fig. S0305 (AIOMFAC_output_0315)

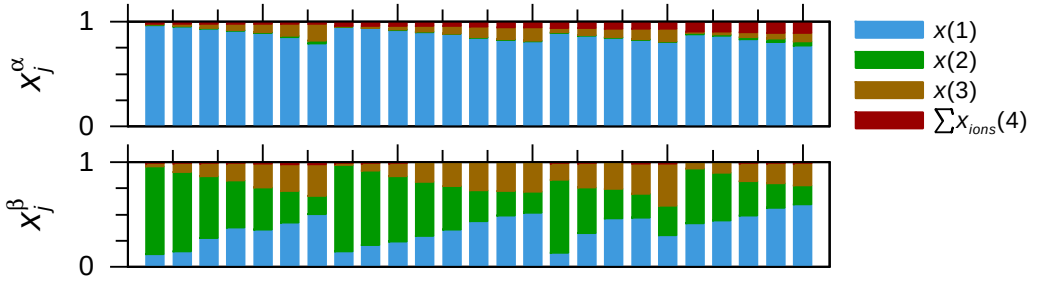
H_2O (1) + 4-Methyl-2-pentanone (2) + Acetic_acid (3) + Na_2SO_4 (4)

Temperature: 308 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)





initial weighting of dataset:

$w^{init}(0315)$ = 1.000

dataset contribution to F_{obj}:

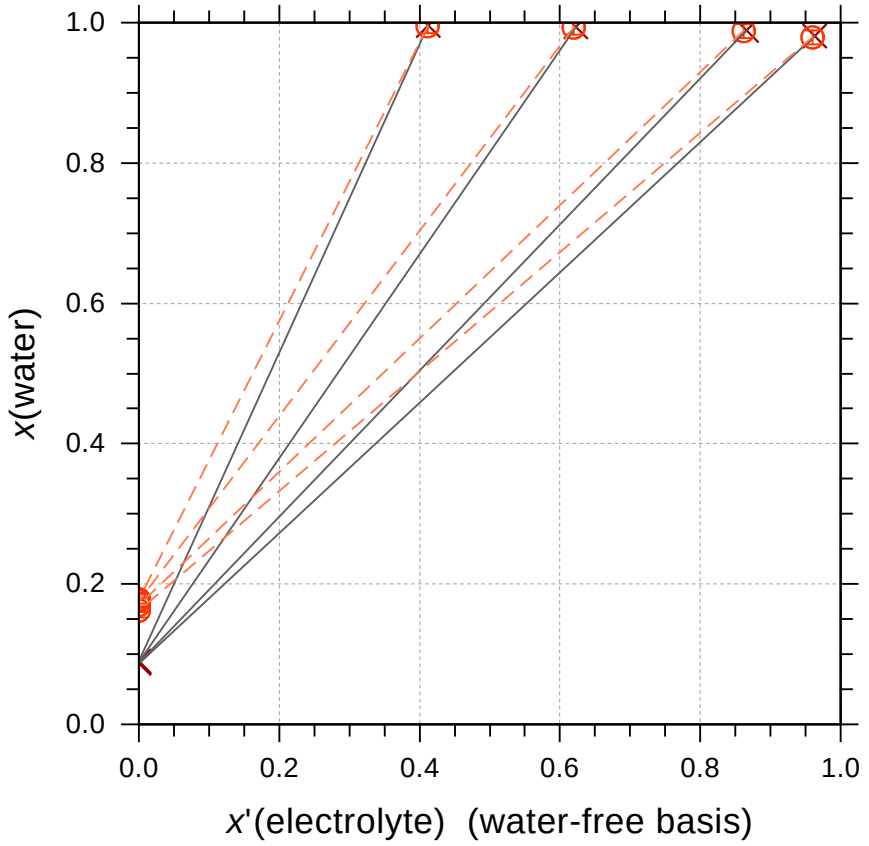
fval(0315) = 1.8778E+00

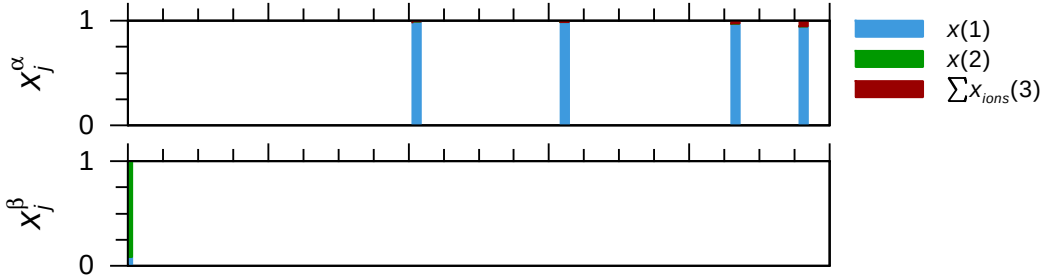
rel. contribution = 0.8930 %

Fig. S0306 (AIOMFAC_output_0355)

H_2O (1) + 4-Methyl-2-pentanone (2) + Na_2SO_4 (3)

Temperature: 298 K





left y-axis:

× Na2SO4+4-Methyl-2-pentanone+Water_LLE_Schunk

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0355) = 1.000

dataset contribution to F_{obj}:

fval(0355) = 2.2259E-01

rel. contribution = 0.1058 %

Fig. S0306a (AIOMFAC_output_0355)

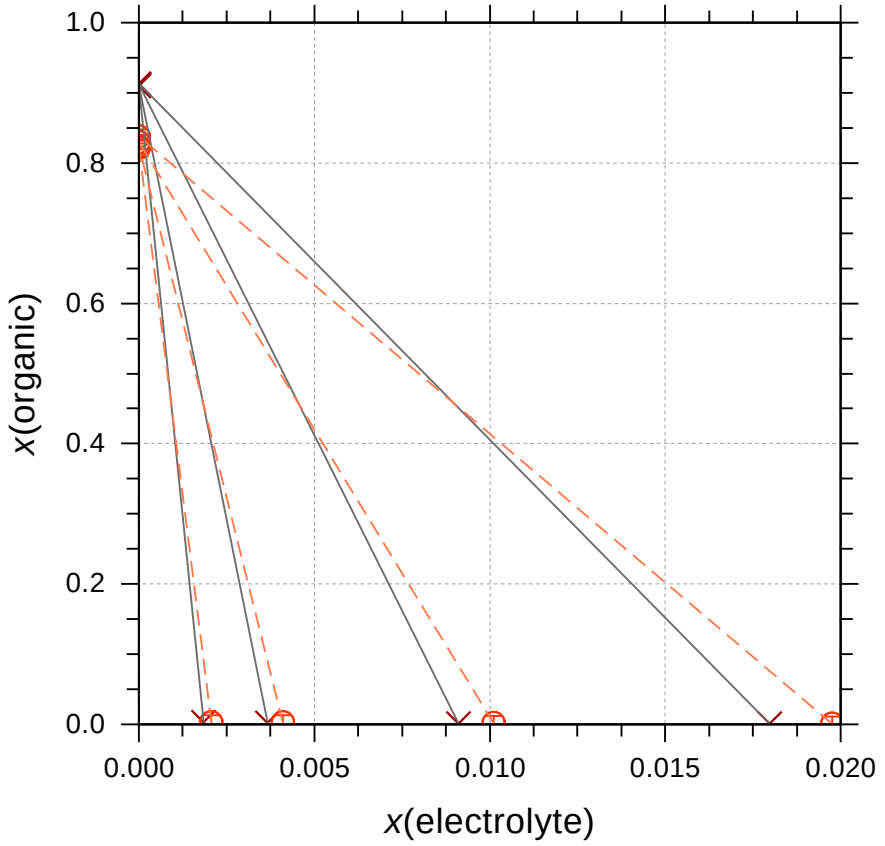
H_2O (1) + 4-Methyl-2-pentanone (2) + Na_2SO_4 (3)

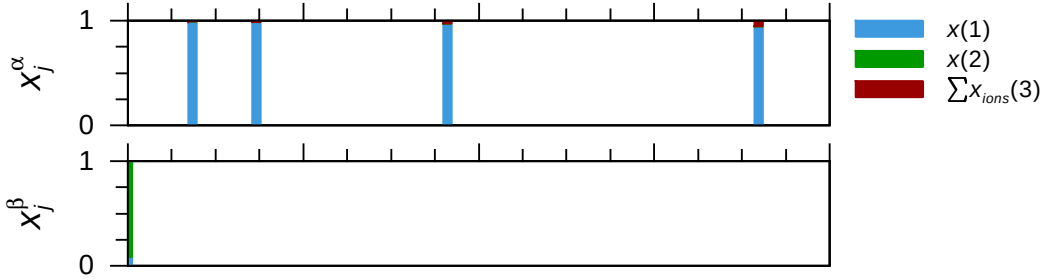
Temperature: 298 K

left y-axis:

× Na2SO4+4-Methyl-2-pentanone+Water_LLE_Schunk

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0355)$ = 1.000

dataset contribution to F_{obj}:

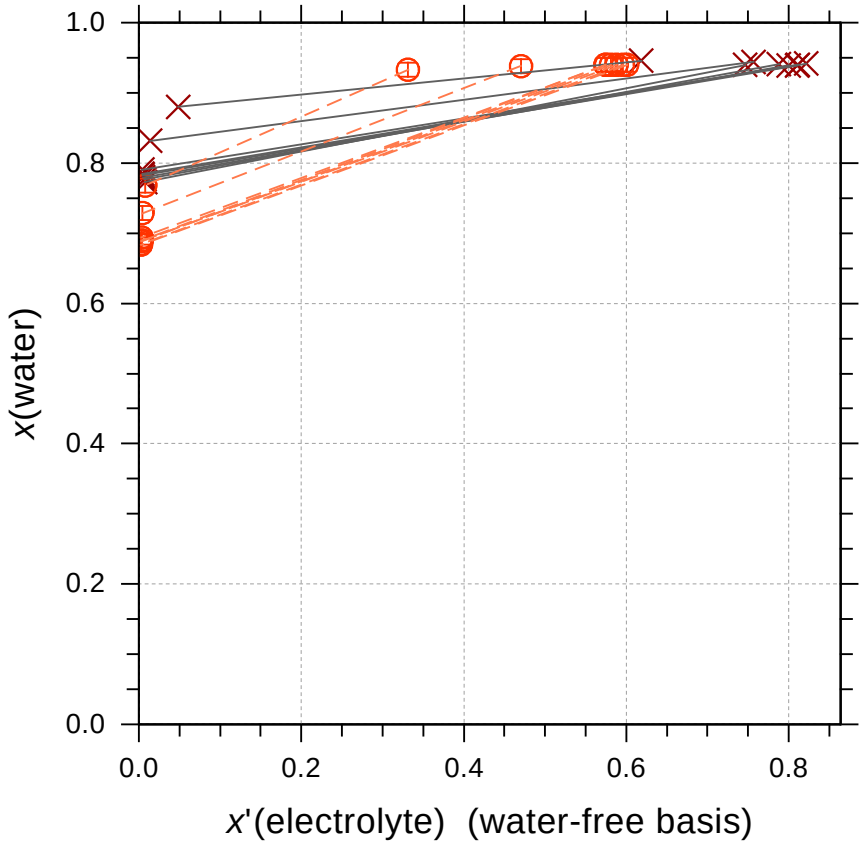
fval(0355) = 2.2259E-01

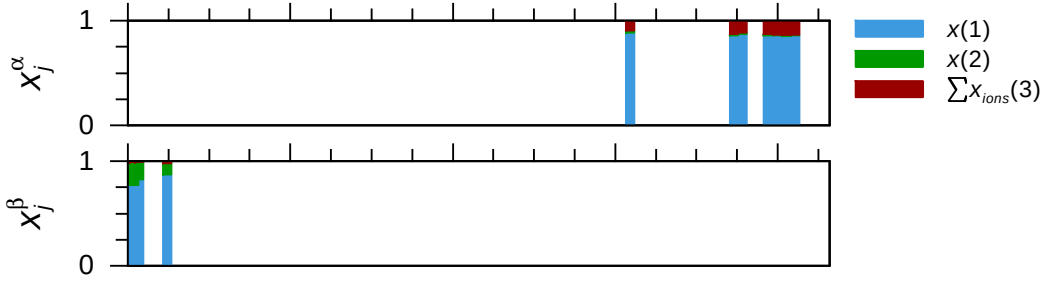
rel. contribution = 0.1058 %

Fig. S0307 (AIOMFAC_output_0925)

H_2O (1) + Acetone (2) + Na_2SO_4 (3)

Temperature range: 303 -- 323 K





left y-axis:

× Na2SO4+Acetone+Water_LLE_Lynn

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0925) = 0.800

dataset contribution to F_{obj}:

fval(0925) = 1.3807E-01

rel. contribution = 0.0657 %

Fig. S0307a (AIOMFAC_output_0925)

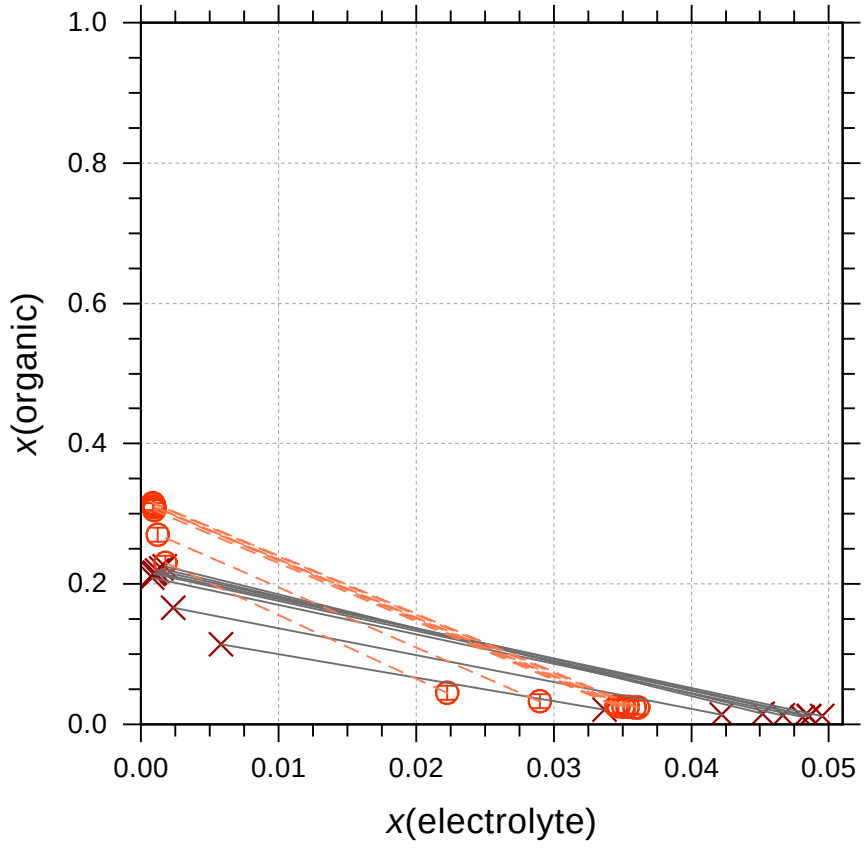
H_2O (1) + Acetone (2) + Na_2SO_4 (3)

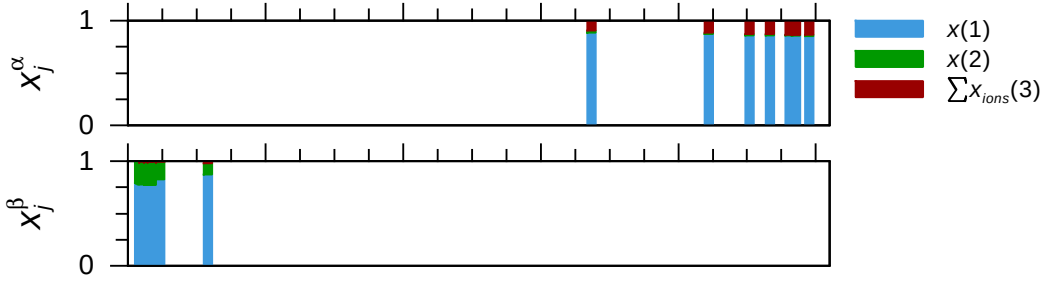
Temperature range: 303 -- 323 K

left y-axis:

× Na2SO4+Acetone+Water_LLE_Lynn

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0925) = 0.800

dataset contribution to F_{obj}:

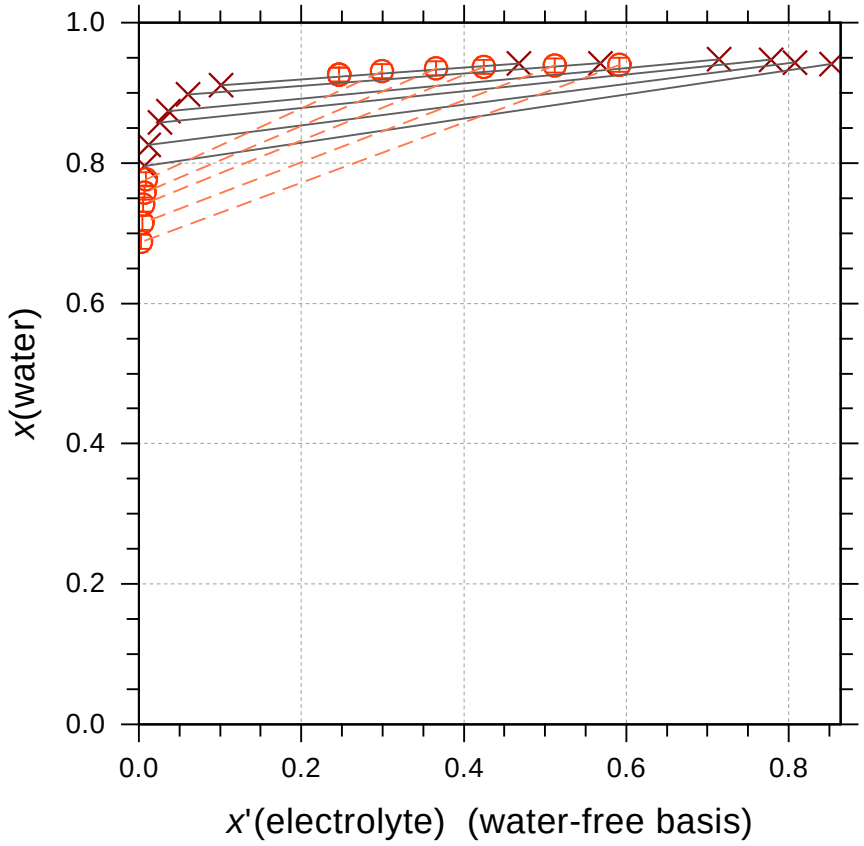
fval(0925) = 1.3807E-01

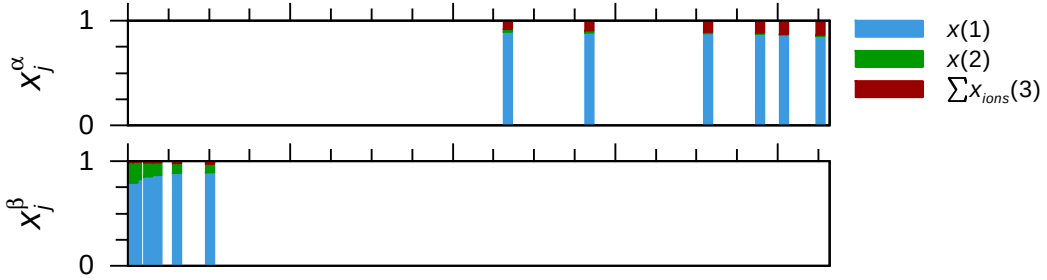
rel. contribution = 0.0657 %

Fig. S0308 (AIOMFAC_output_0926)

H_2O (1) + Acetone (2) + Na_2SO_4 (3)

Temperature: 308 K





left y-axis:

× Na2SO4+Acetone+Water_LLE_Lynn_308K

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0926) = 0.800

dataset contribution to F_{obj}:

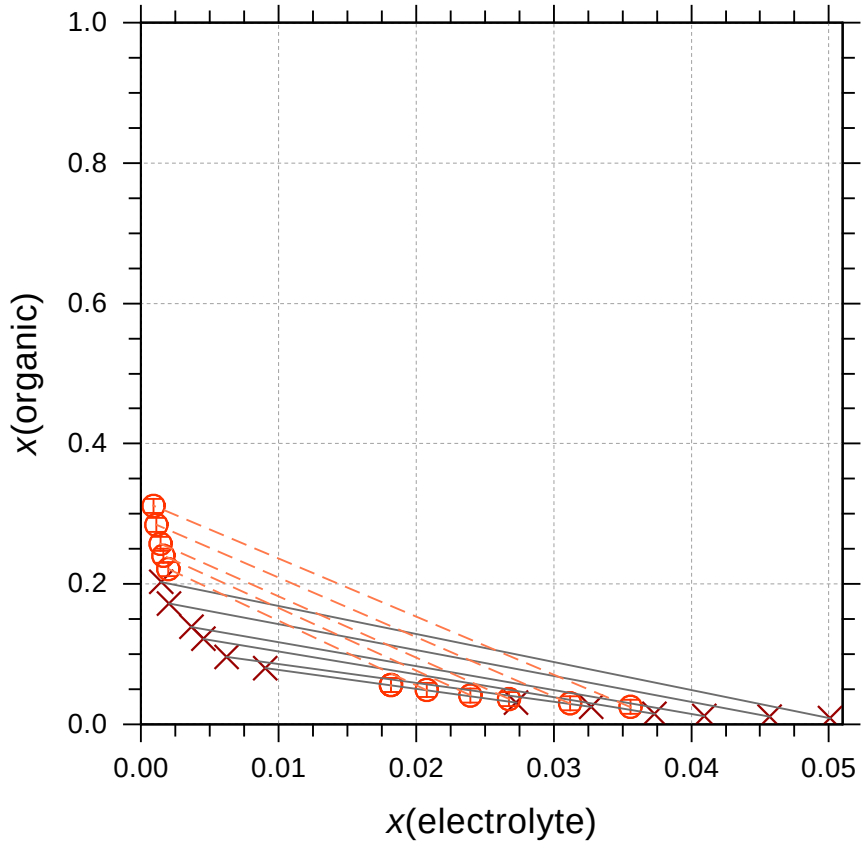
fval(0926) = 1.8045E-01

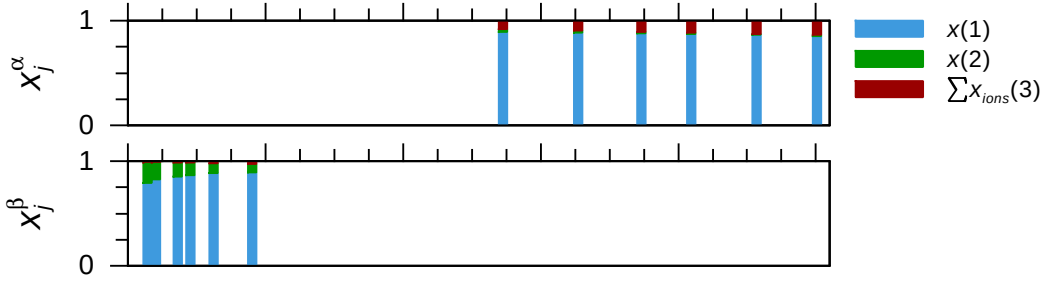
rel. contribution = 0.0858 %

Fig. S0308a (AIOMFAC_output_0926)

H_2O (1) + Acetone (2) + Na_2SO_4 (3)

Temperature: 308 K





left y-axis:

× Na2SO4+Acetone+Water_LLE_Lynn_308K

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0926) = 0.800

dataset contribution to F_{obj}:

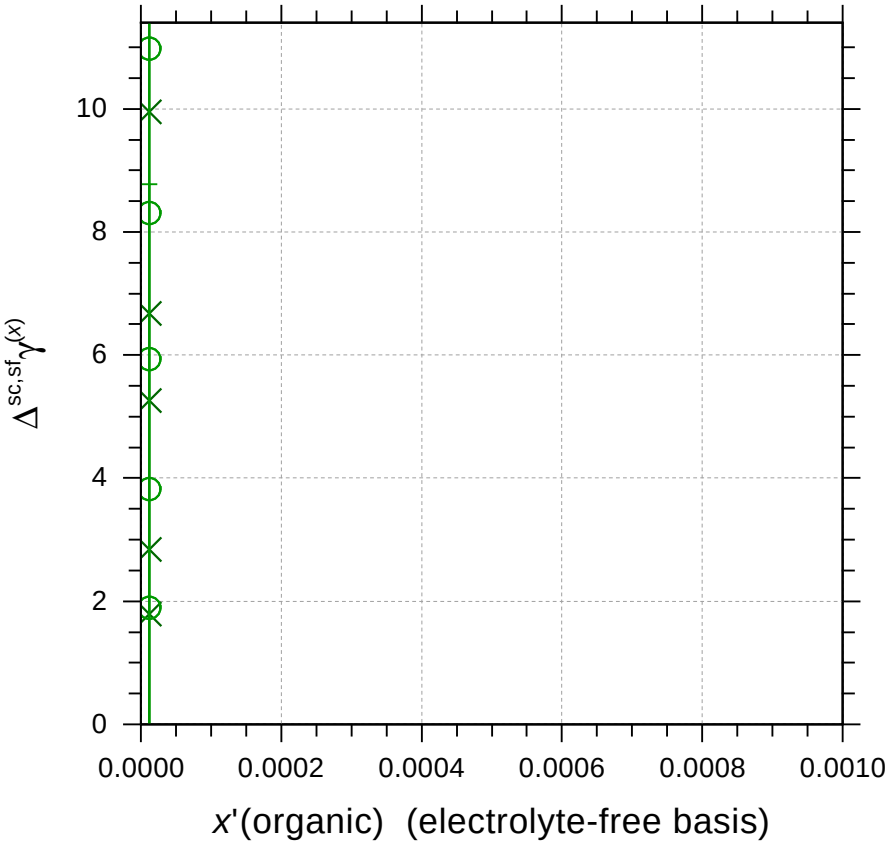
fval(0926) = 1.8045E-01

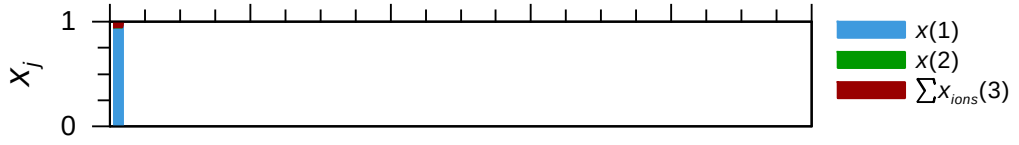
rel. contribution = 0.0858 %

Fig. S0309 (AIOMFAC_output_0989)

H_2O (1) + Acetone (2) + Na_2SO_4 (3)

Temperature: 323 K



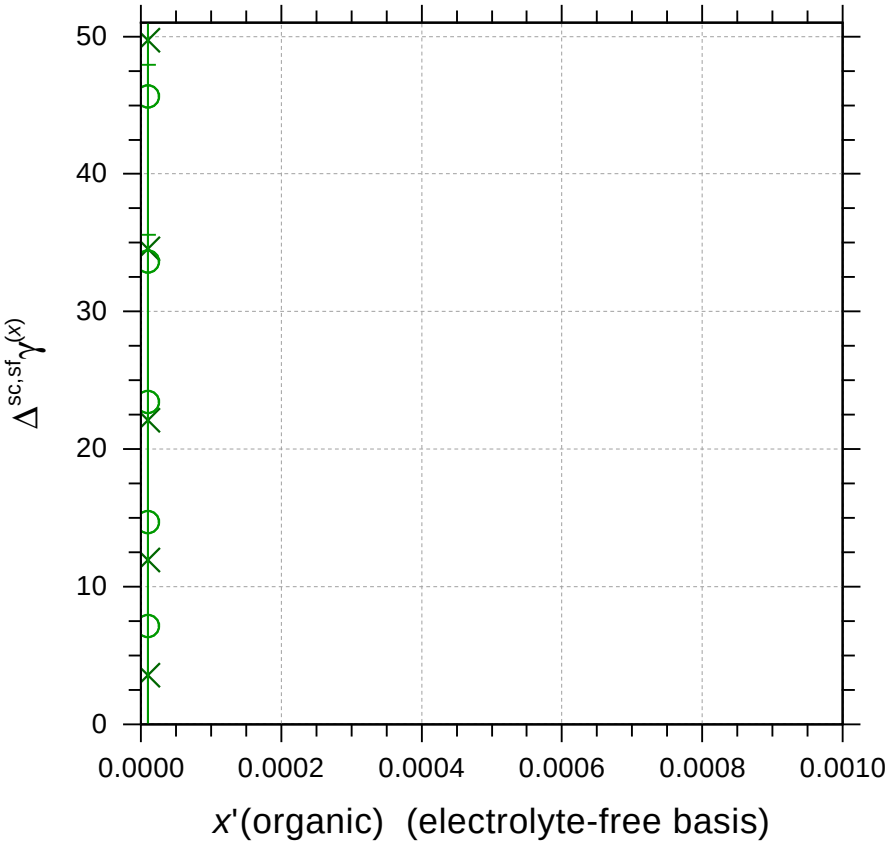


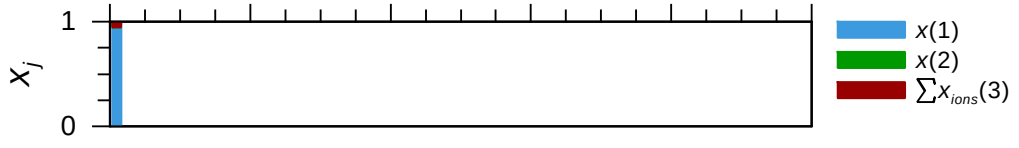
initial weighting of dataset:
$w^{init}(0989)$ = 0.100
dataset contribution to F_{obj}:
fval(0989) = 2.0003E-03
rel. contribution = 0.0010 %

Fig. S0310 (AIOMFAC_output_0990)

H_2O (1) + 2-Butanone (2) + Na_2SO_4 (3)

Temperature: 323 K



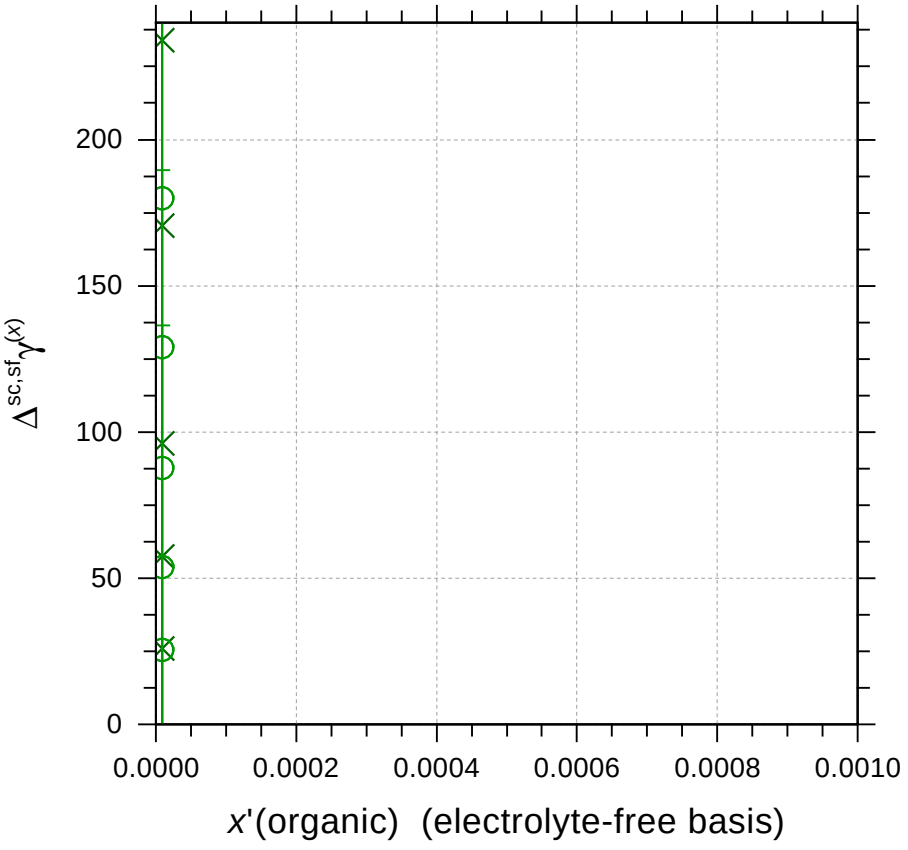


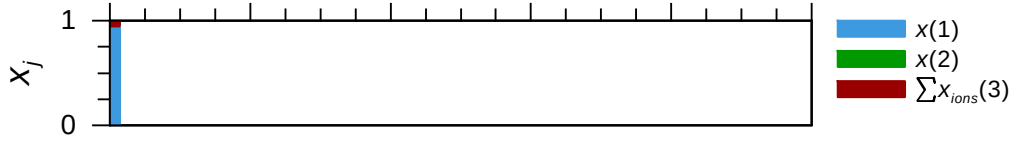
initial weighting of dataset:
$w^{init}(0990)$ = 0.100
dataset contribution to F_{obj}:
fval(0990) = 1.7249E-03
rel. contribution = 0.0008 %

Fig. S0311 (AIOMFAC_output_0991)

H_2O (1) + 2-Pentanone (2) + Na_2SO_4 (3)

Temperature: 323 K



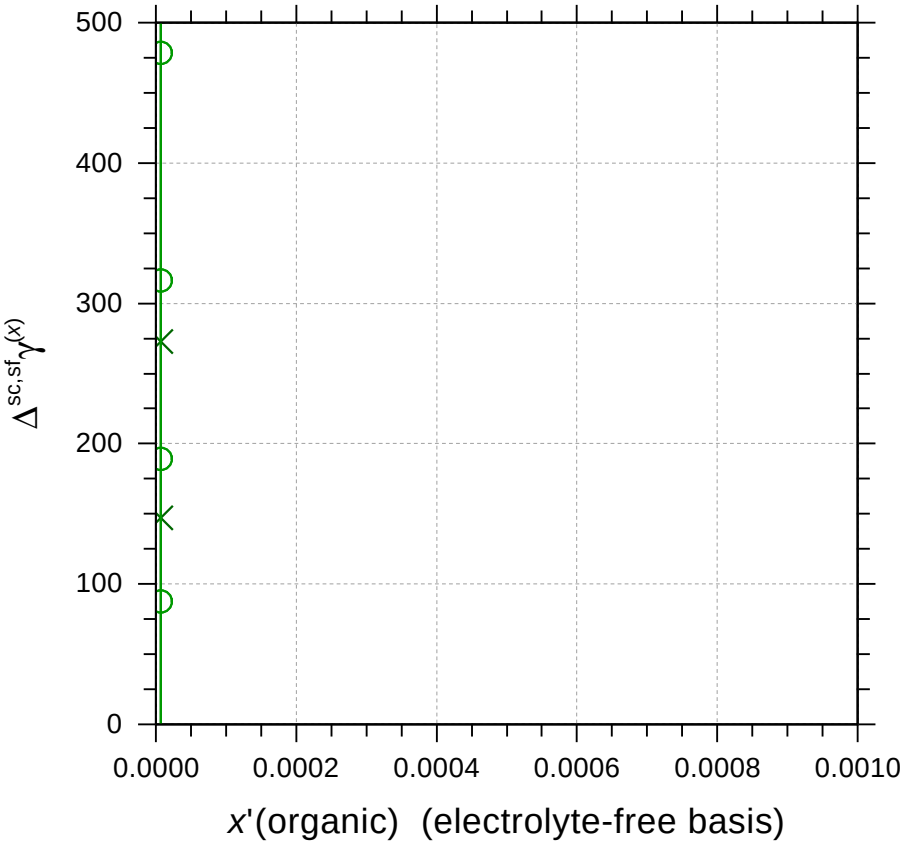


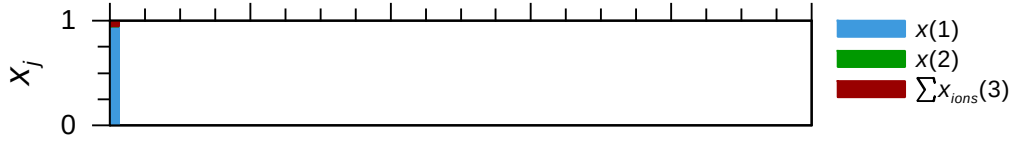
initial weighting of dataset:
$w^{init}(0991)$ = 0.100
dataset contribution to F_{obj}:
fval(0991) = 2.4618E-03
rel. contribution = 0.0012 %

Fig. S0312 (AIOMFAC_output_0992)

H_2O (1) + 2-Hexanone (2) + Na_2SO_4 (3)

Temperature: 323 K





left y-axis:

× Na2SO4+2-Hexanone+Water_VLE_Chai (EXP, org.)

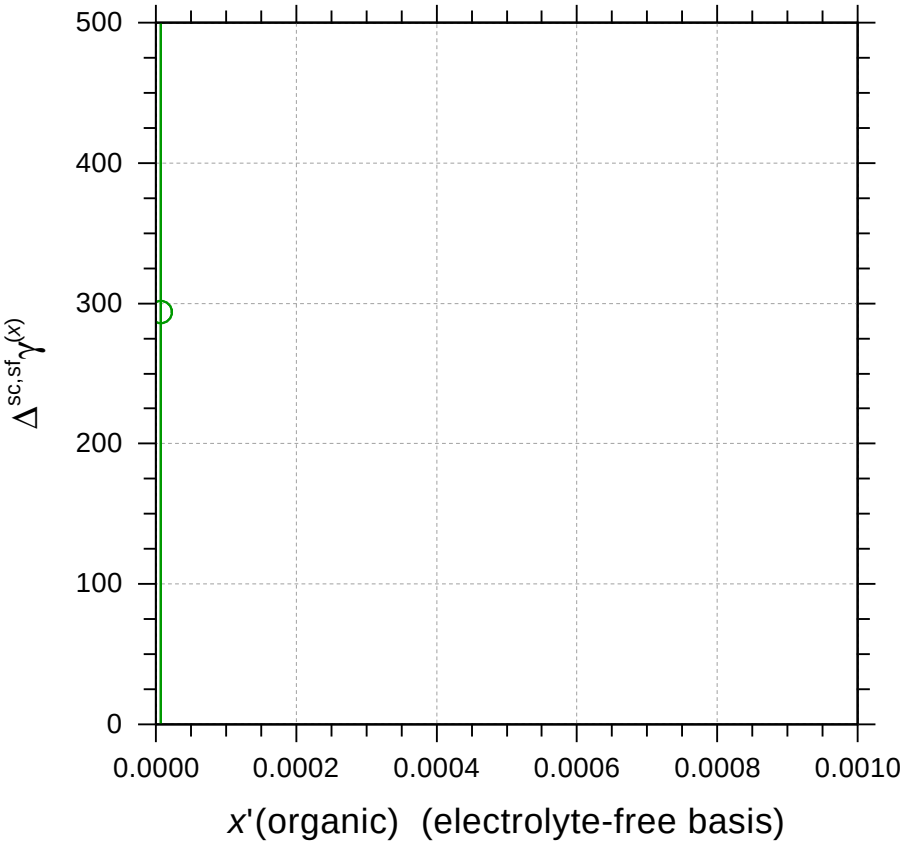
○ AIOMFAC $\Delta^{sc,sf}\gamma^{(x)}_{org.}$

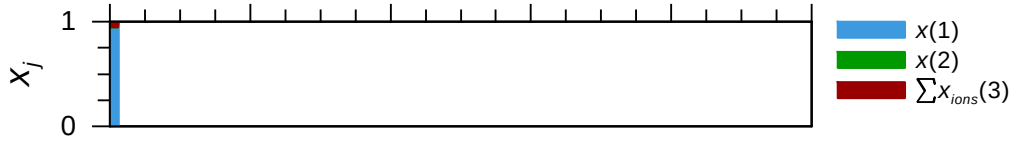
initial weighting of dataset:
$w^{init}(0992)$ = 0.100
dataset contribution to F_{obj}:
fval(0992) = 8.9005E-03
rel. contribution = 0.0042 %

Fig. S0313 (AIOMFAC_output_0993)

H_2O (1) + 2-Heptanone (2) + Na_2SO_4 (3)

Temperature: 323 K





left y-axis:

× Na2SO4+2-Heptanone+Water_VLE_Chai (EXP, org.)

○ AIOMFAC $\Delta^{sc,sf}\gamma^{(x)}_{org.}$

initial weighting of dataset:
$w^{init}(0993)$ = 0.100
dataset contribution to F_{obj}:
fval(0993) = 2.0450E-02
rel. contribution = 0.0097 %

Fig. S0314 (AIOMFAC_output_0344)

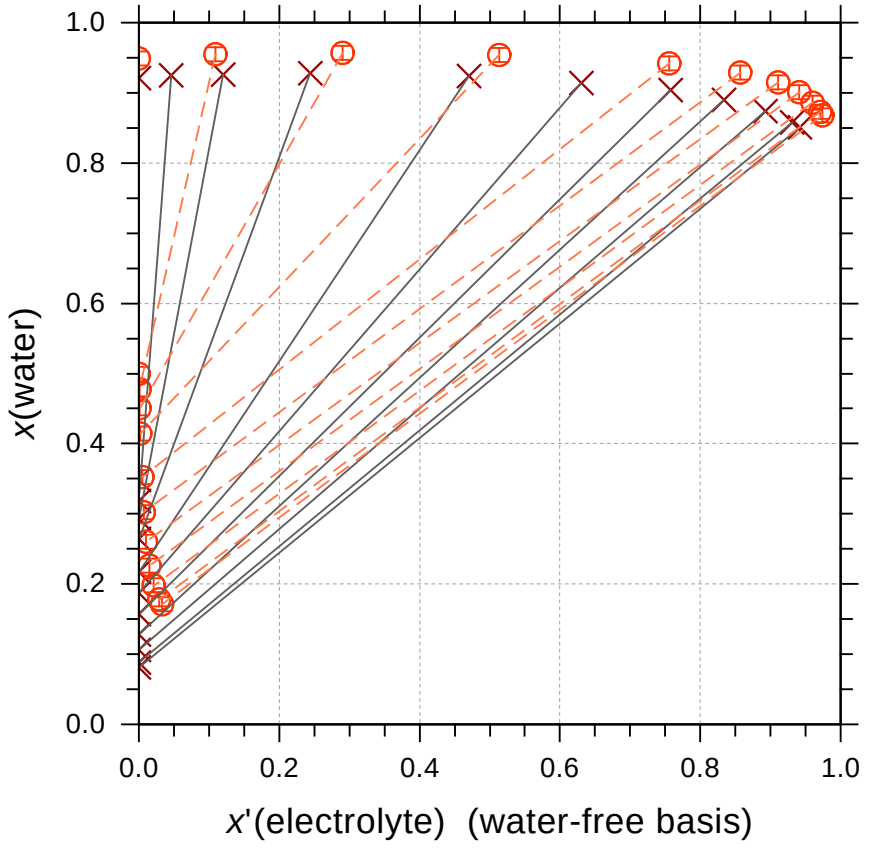
H_2O (1) + 2-Butanone (2) + NaBr (3)

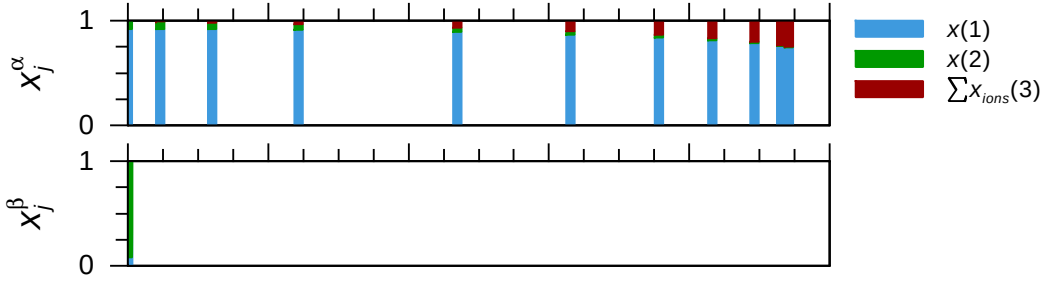
Temperature: 298 K

left y-axis:

× NaBr+Butanone+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0344)$ = 1.000

dataset contribution to F_{obj}:

fval(0344) = 1.7930E+00

rel. contribution = 0.8526 %

Fig. S0314a (AIOMFAC_output_0344)

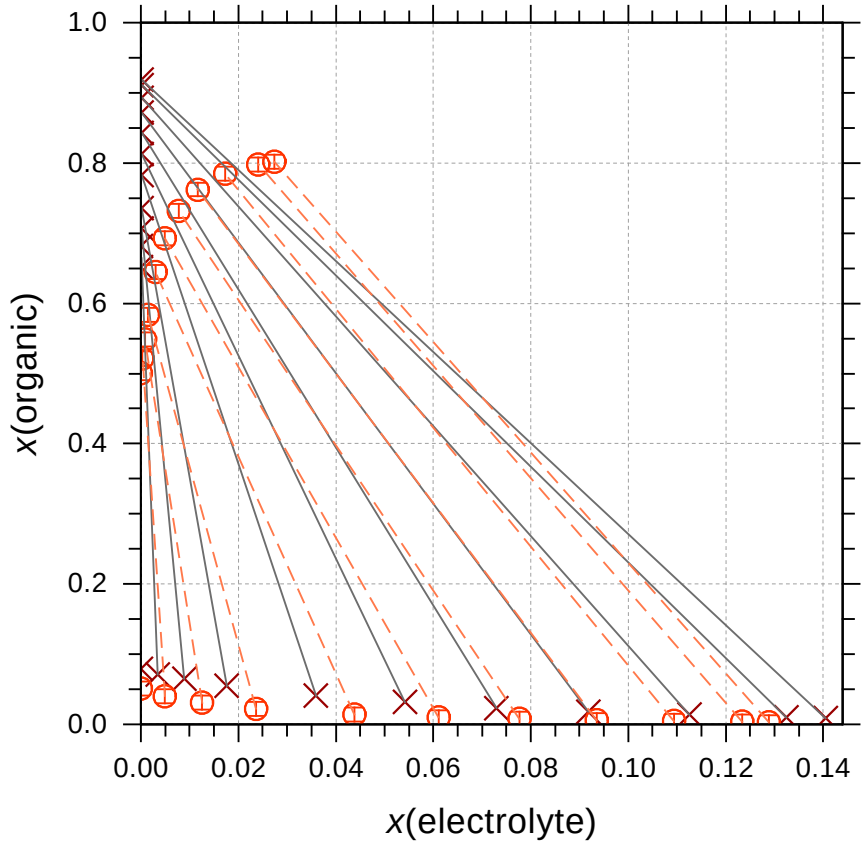
H_2O (1) + 2-Butanone (2) + NaBr (3)

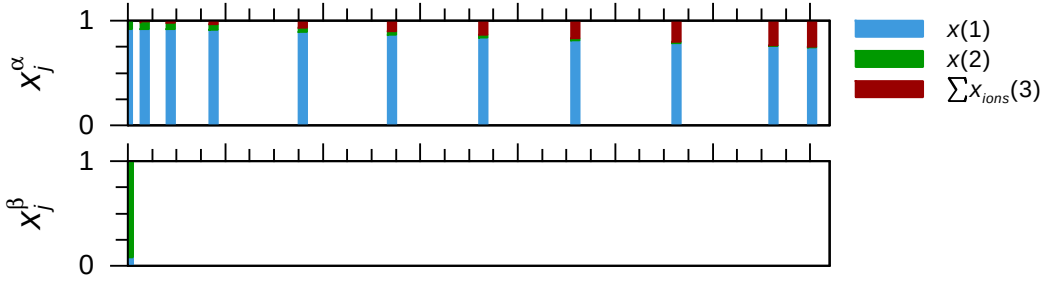
Temperature: 298 K

left y-axis:

× NaBr+Butanone+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0344) = 1.000

dataset contribution to F_{obj}:

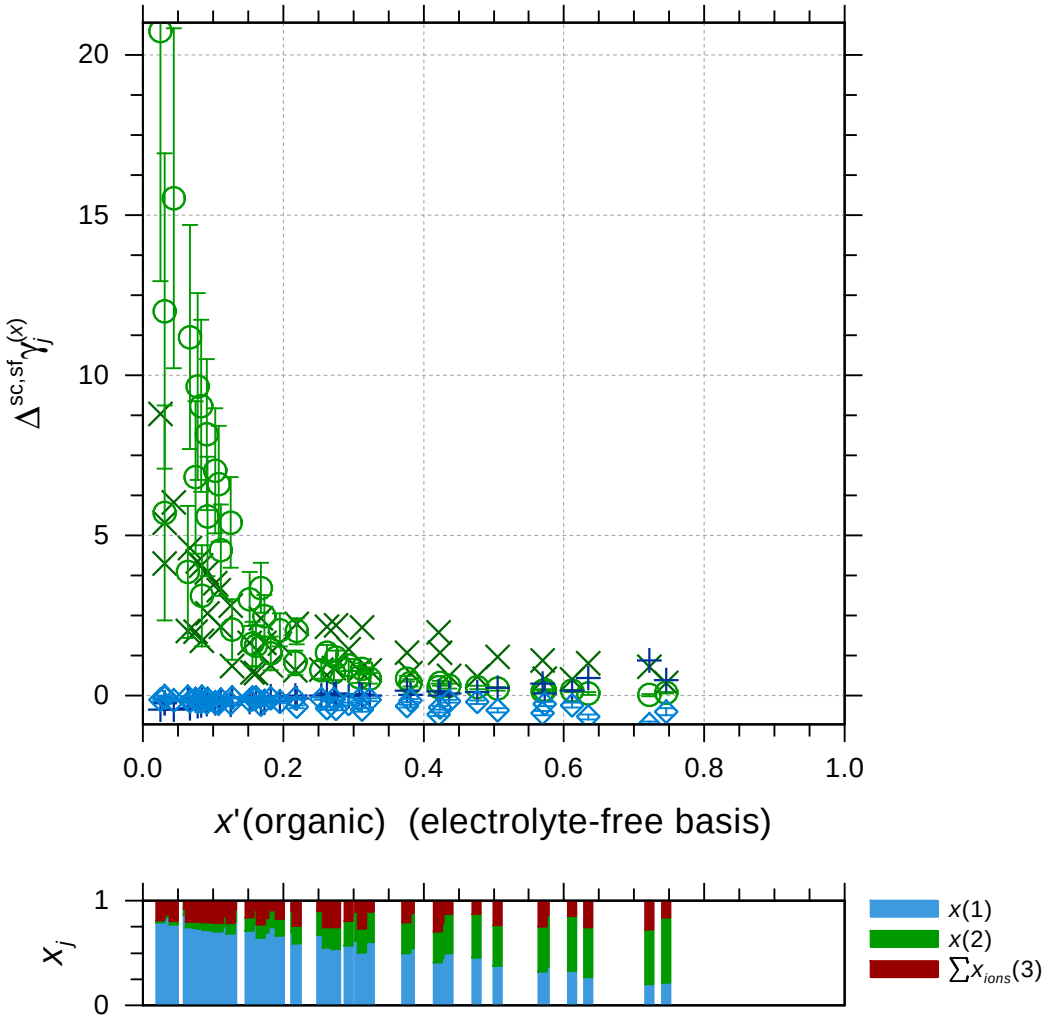
fval(0344) = 1.7930E+00

rel. contribution = 0.8526 %

Fig. S0315 (AIOMFAC_output_0358)

H_2O (1) + Acetone (2) + NaBr (3)

Temperature range: 324 -- 356 K



initial weighting of dataset:
$w^{init}(0358)$ = 0.500
dataset contribution to F_{obj}:
fval(0358) = 1.3663E+00
rel. contribution = 0.6497 %

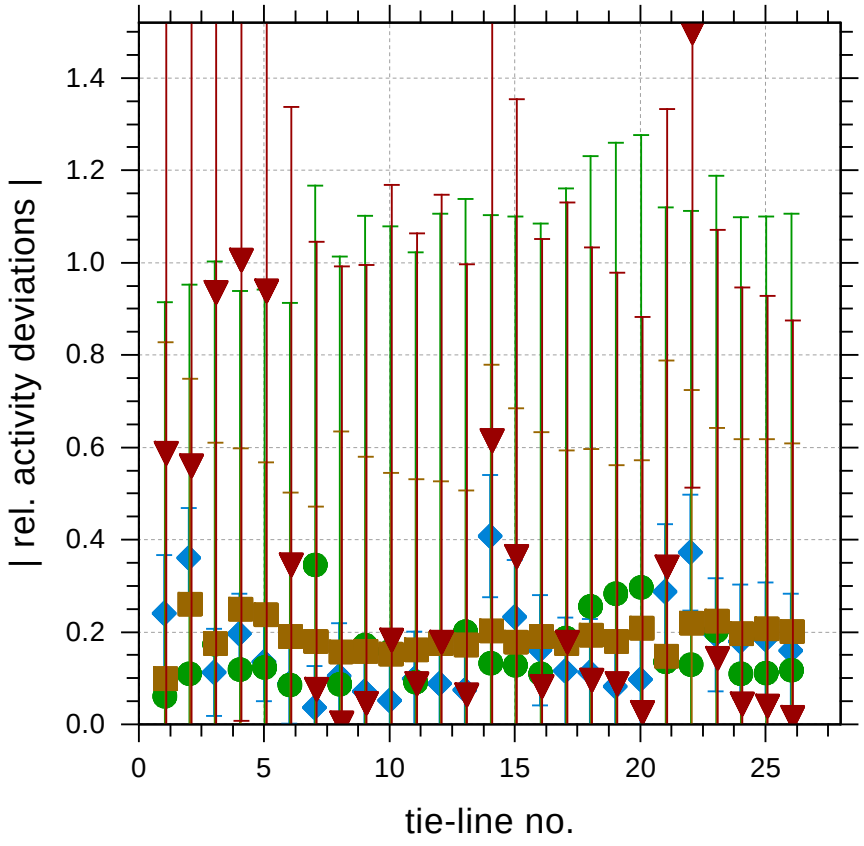
Fig. S0316 (AIOMFAC_output_0299)

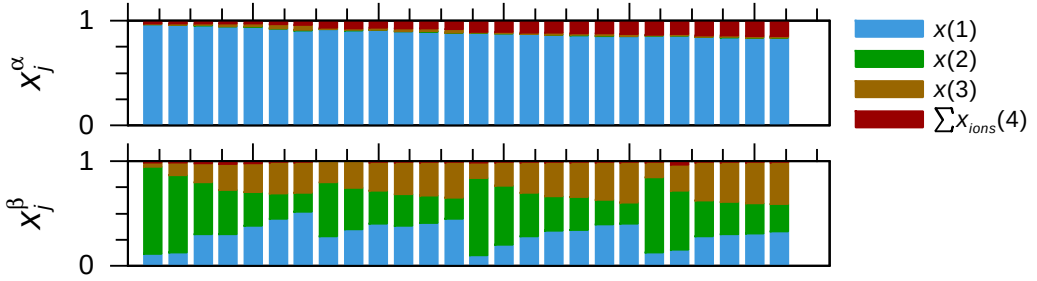
H_2O (1) + 4-Methyl-2-pentanone (2) + Propanoic_acid (3) + NaCl (4)

Temperature: 308 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



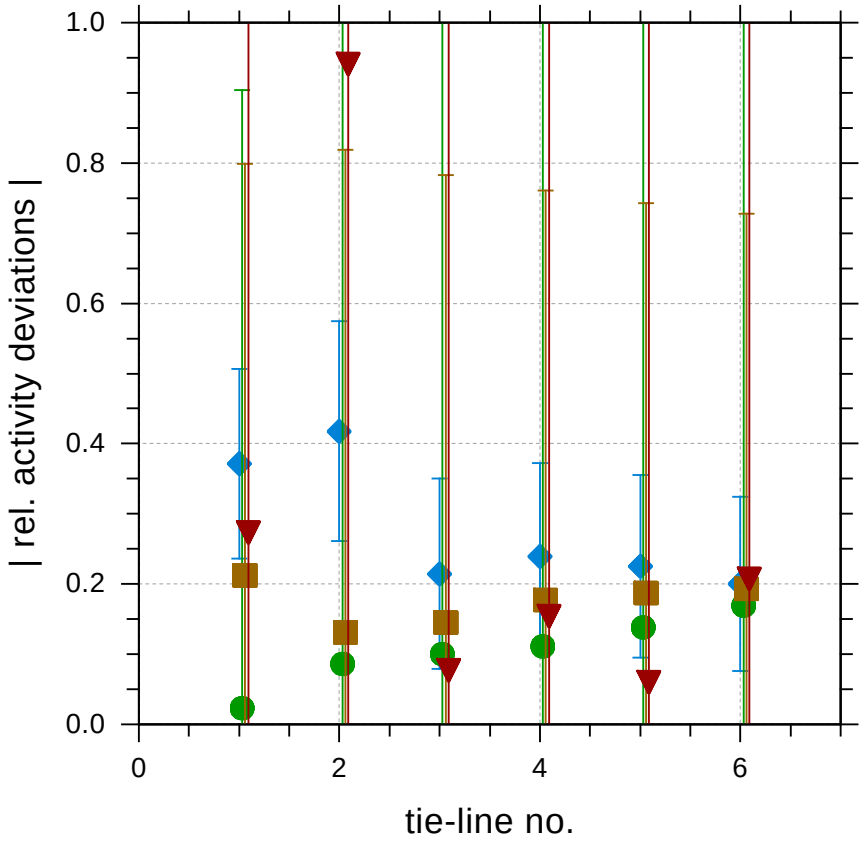


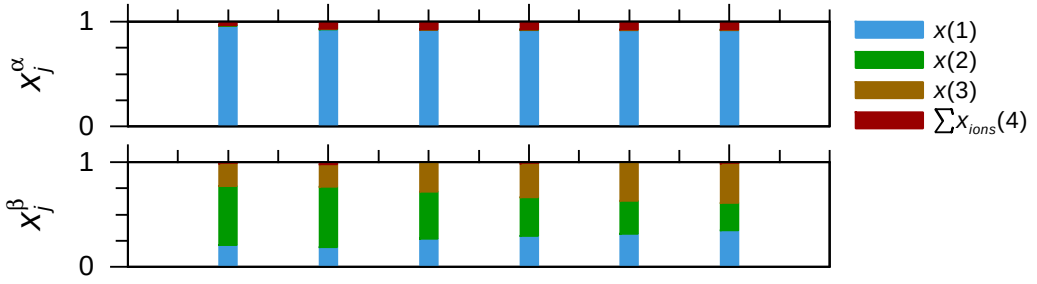
initial weighting of dataset:
$w^{init}(0299)$ = 1.000
dataset contribution to F_{obj}:
fval(0299) = 1.7795E+00
rel. contribution = 0.8462 %

Fig. S0317 (AIOMFAC_output_0306)

H_2O (1) + 4-Methyl-2-pentanone (2) + Butyric_acid (3) + NaCl (4)

Temperature: 308 K





left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

initial weighting of dataset:
w^{init}(0306) = 1.000
dataset contribution to F_{obj}:
fval(0306) = 1.5065E+00
rel. contribution = 0.7164 %

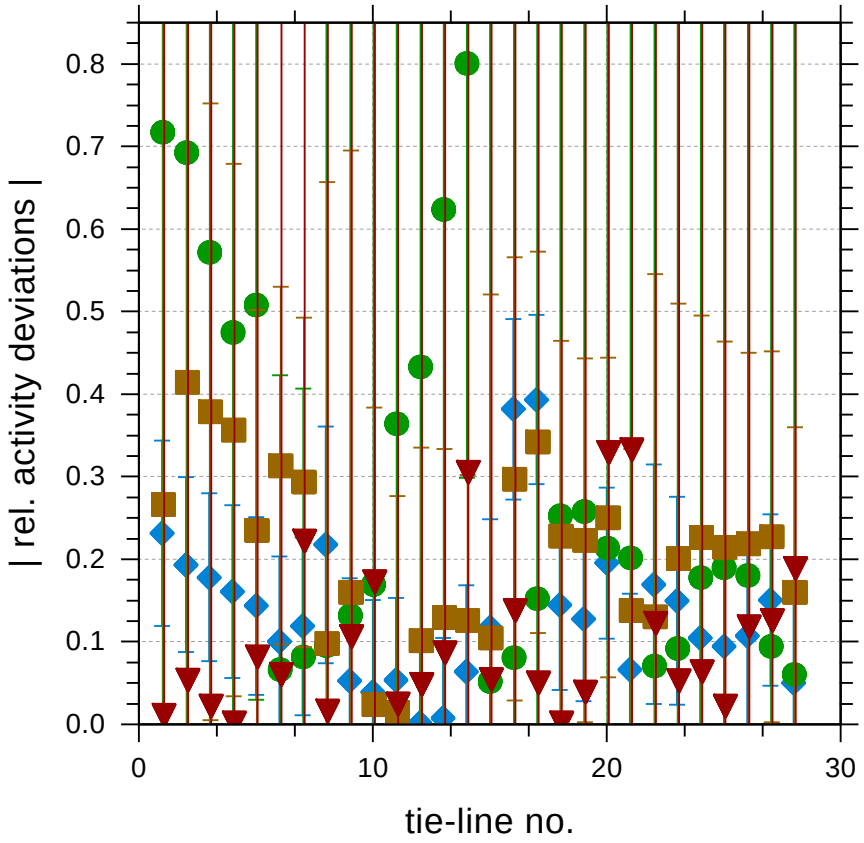
Fig. S0318 (AIOMFAC_output_0313)

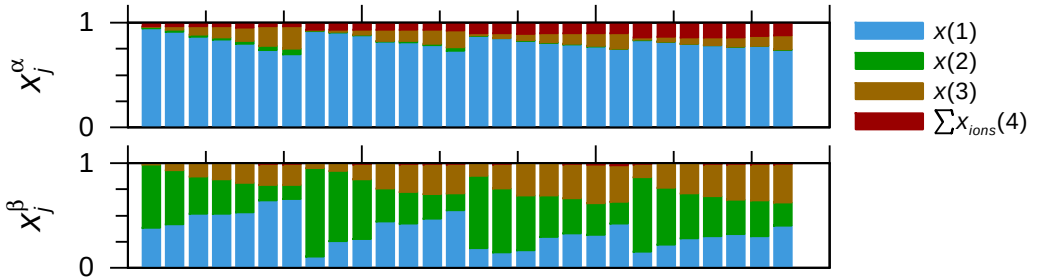
H_2O (1) + 4-Methyl-2-pentanone (2) + Acetic_acid (3) + NaCl (4)

Temperature: 308 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



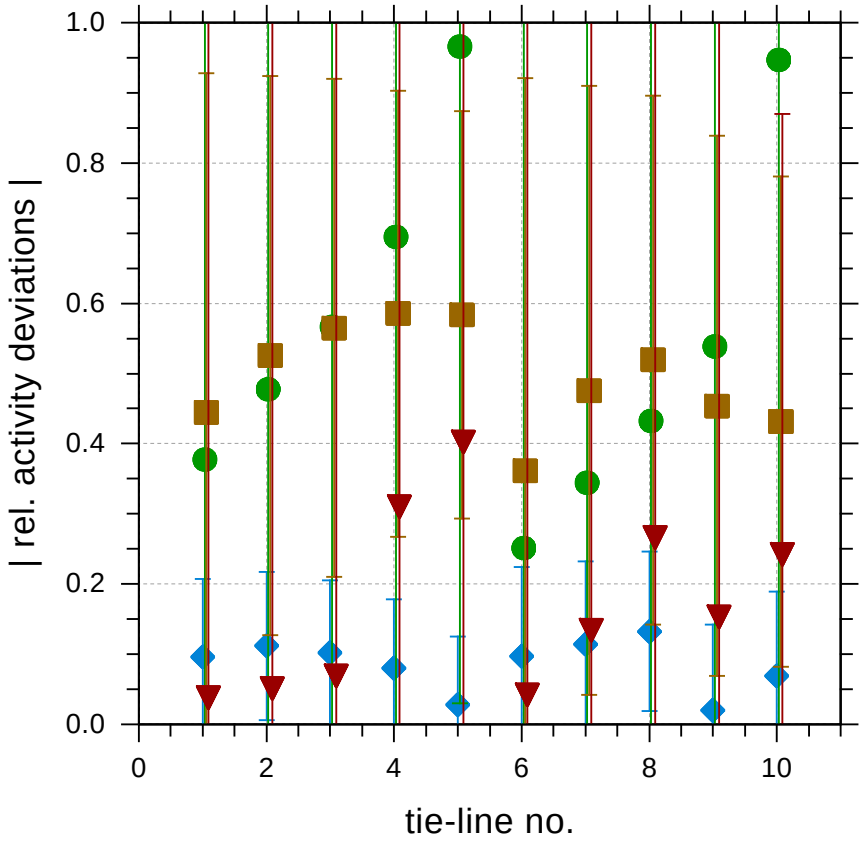


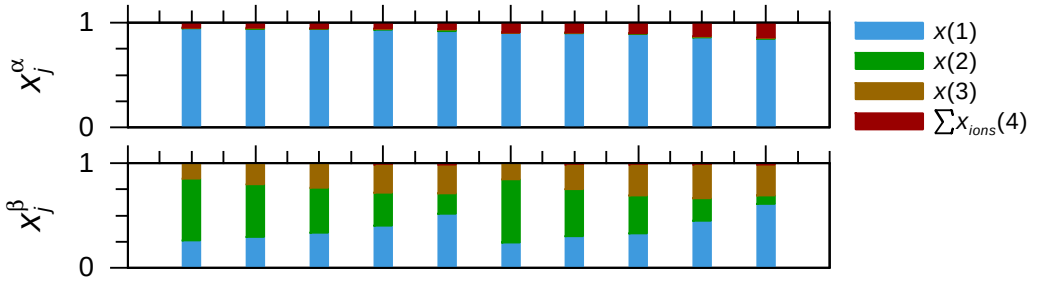
initial weighting of dataset:
$w^{init}(0313)$ = 1.000
dataset contribution to F_{obj}:
fval(0313) = 1.1428E+00
rel. contribution = 0.5434 %

Fig. S0319 (AIOMFAC_output_0317)

H_2O (1) + 4-Methyl-2-pentanone (2) + Propanoic_acid (3) + NaCl (4)

Temperature: 298 K





initial weighting of dataset:
$w^{init}(0317)$ = 1.000
dataset contribution to F_{obj}:
fval(0317) = 3.3400E+00
rel. contribution = 1.5883 %

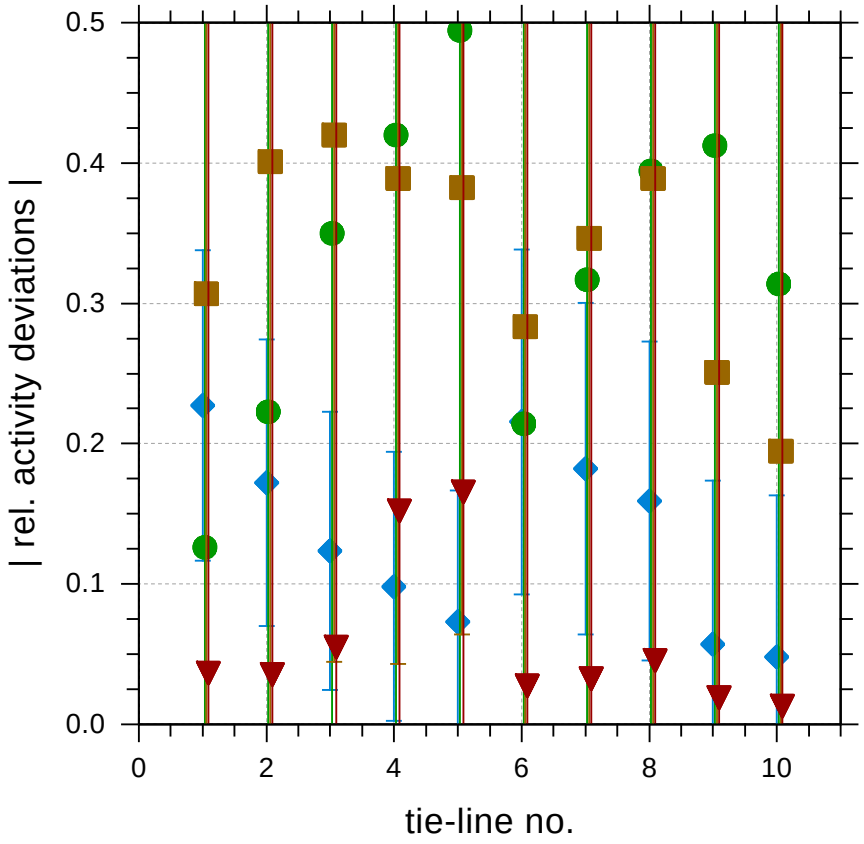
Fig. S0320 (AIOMFAC_output_0319)

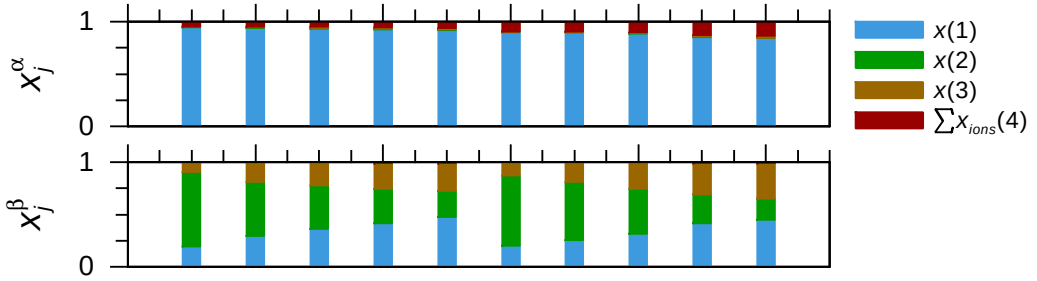
H_2O (1) + 3-Methyl-2-butanone (2) + Propanoic_acid (3) + NaCl (4)

Temperature: 298 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



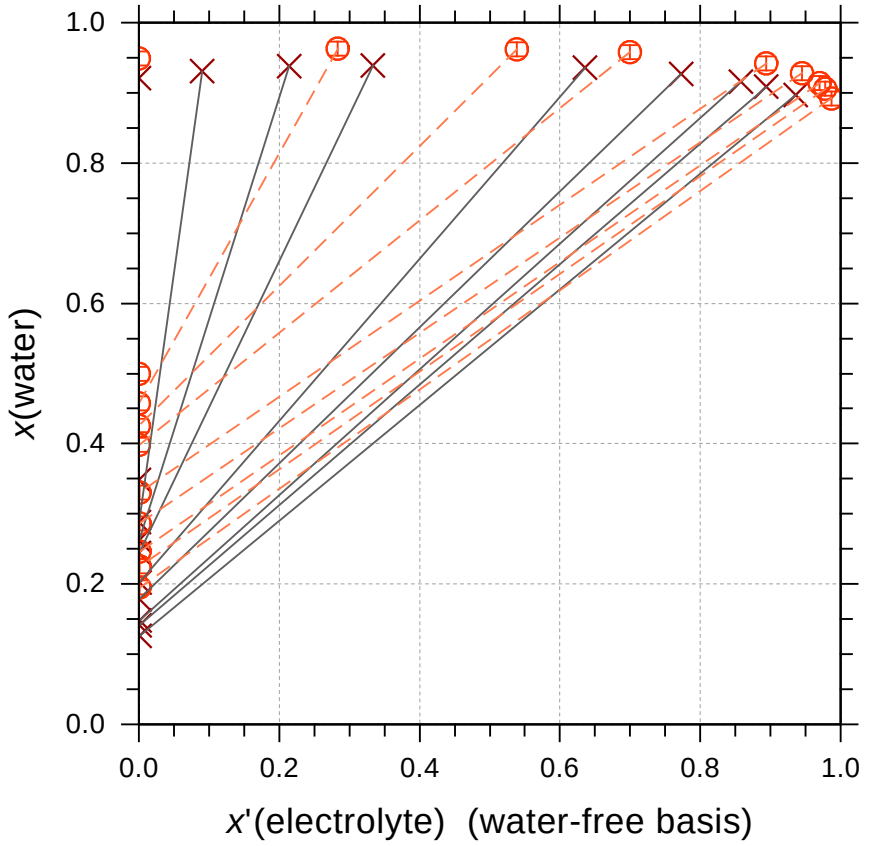


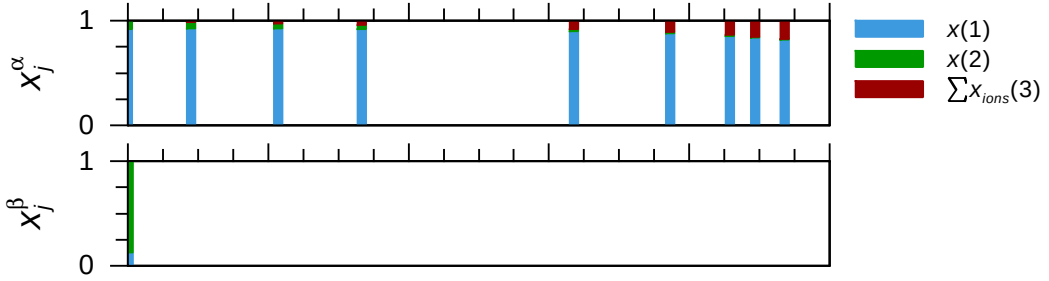
initial weighting of dataset:
w^{init}(0319) = 1.000
dataset contribution to F_{obj}:
fval(0319) = 1.3215E+00
rel. contribution = 0.6284 %

Fig. S0321 (AIOMFAC_output_0325)

H_2O (1) + 2-Butanone (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl+Butanone+Water_LLE_Li

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0325) = 1.000

dataset contribution to F_{obj}:

fval(0325) = 7.4990E-01

rel. contribution = 0.3566 %

Fig. S0321a (AIOMFAC_output_0325)

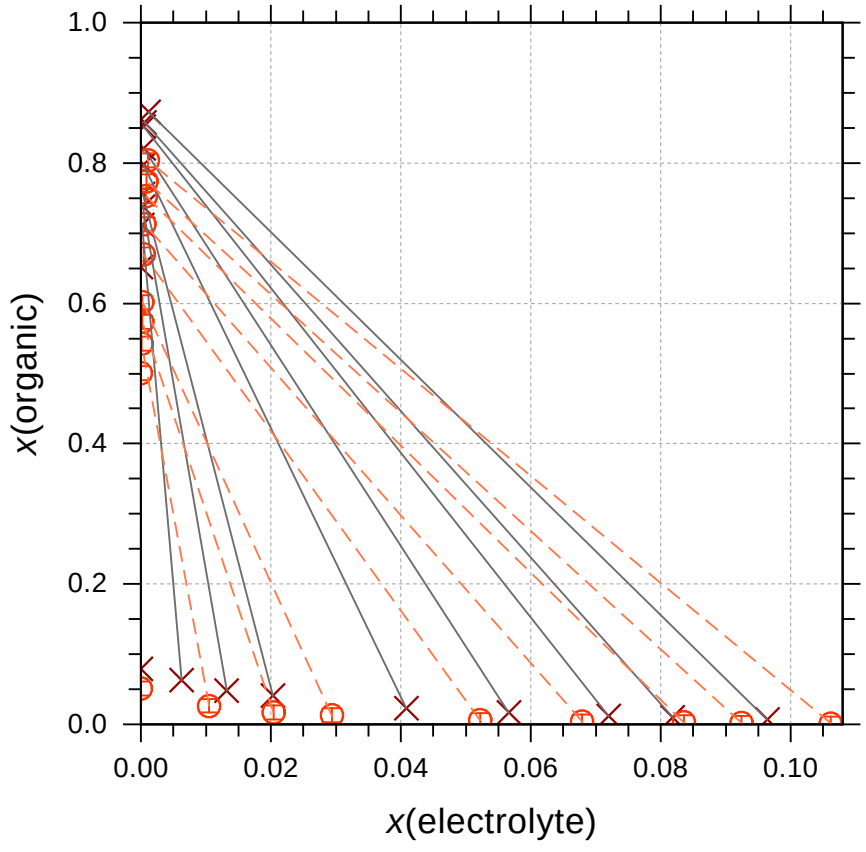
H_2O (1) + 2-Butanone (2) + NaCl (3)

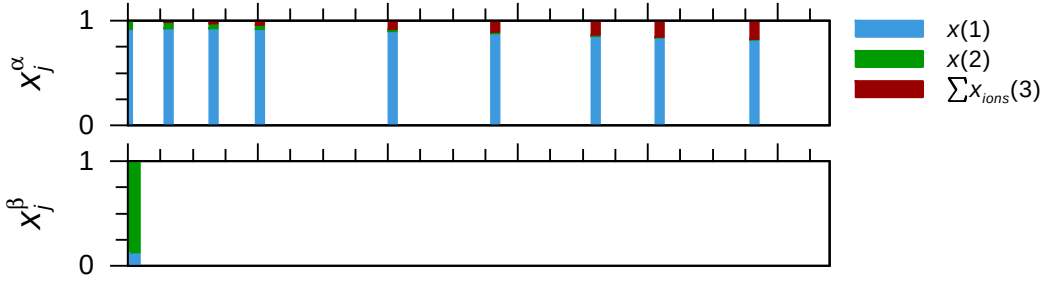
Temperature: 298 K

left y-axis:

× NaCl+Butanone+Water_LLE_Li

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0325) = 1.000

dataset contribution to F_{obj}:

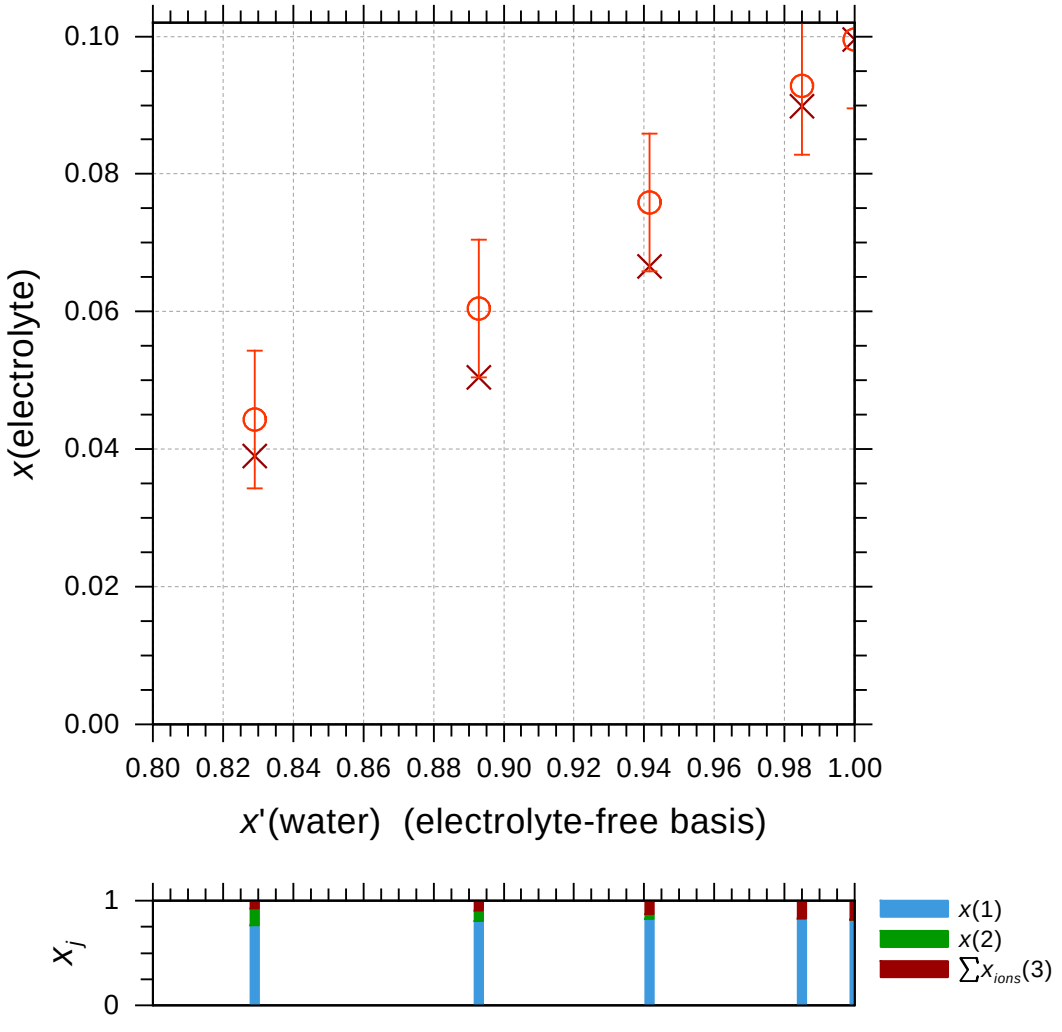
fval(0325) = 7.4990E-01

rel. contribution = 0.3566 %

Fig. S0322 (AIOMFAC_output_0351)

H_2O (1) + Acetone (2) + NaCl (3)

Temperature: 293 K

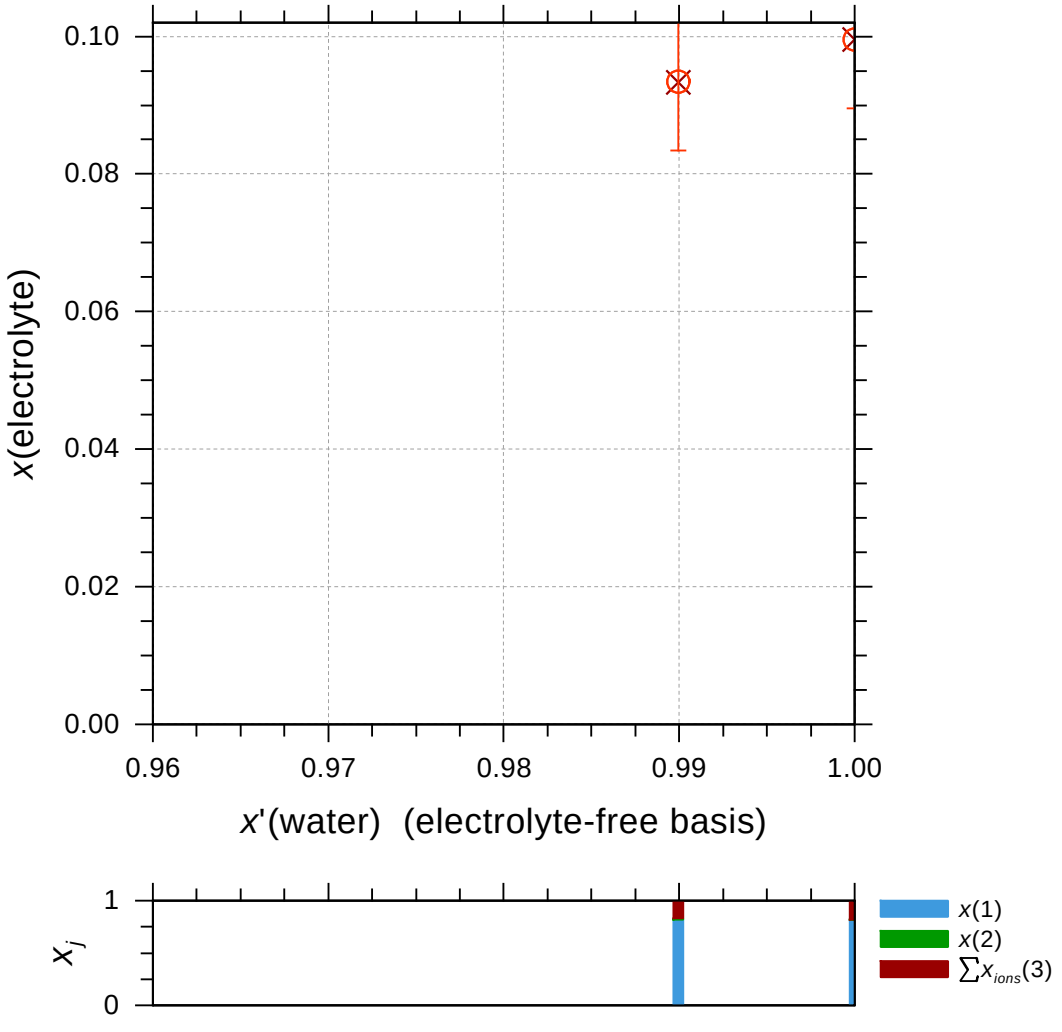


initial weighting of dataset:
w^{init}(0351) = 1.000
dataset contribution to F_{obj}:
fval(0351) = 5.5219E-02
rel. contribution = 0.0263 %

Fig. S0323 (AIOMFAC_output_0352)

H_2O (1) + 2-Butanone (2) + NaCl (3)

Temperature: 293 K

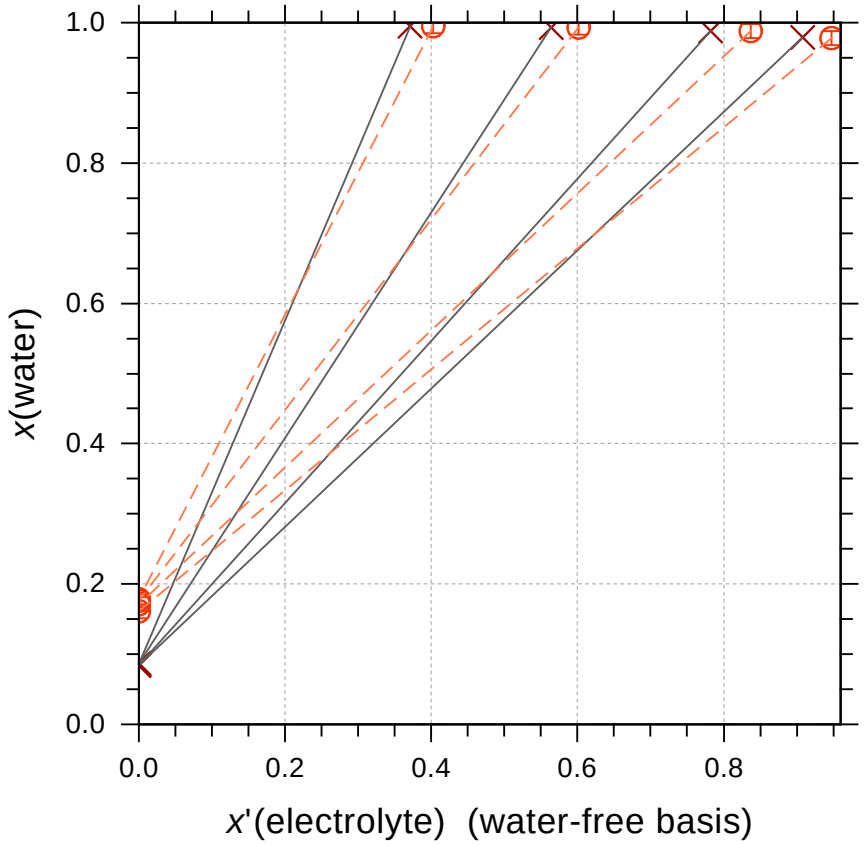


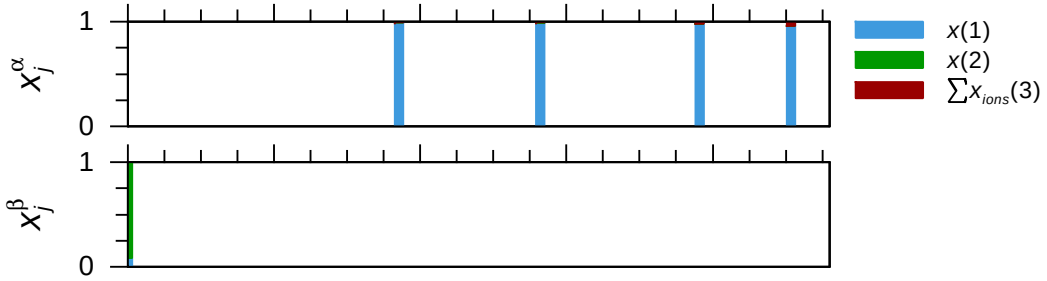
initial weighting of dataset:
$w^{init}(0352)$ = 1.000
dataset contribution to F_{obj}:
fval(0352) = 5.5362E-08
rel. contribution = 0.0000 %

Fig. S0324 (AIOMFAC_output_0353)

H_2O (1) + 4-Methyl-2-pentanone (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl+4-Methyl-2-pentanone+Water_LLE_Schunk

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0353) = 1.000

dataset contribution to F_{obj}:

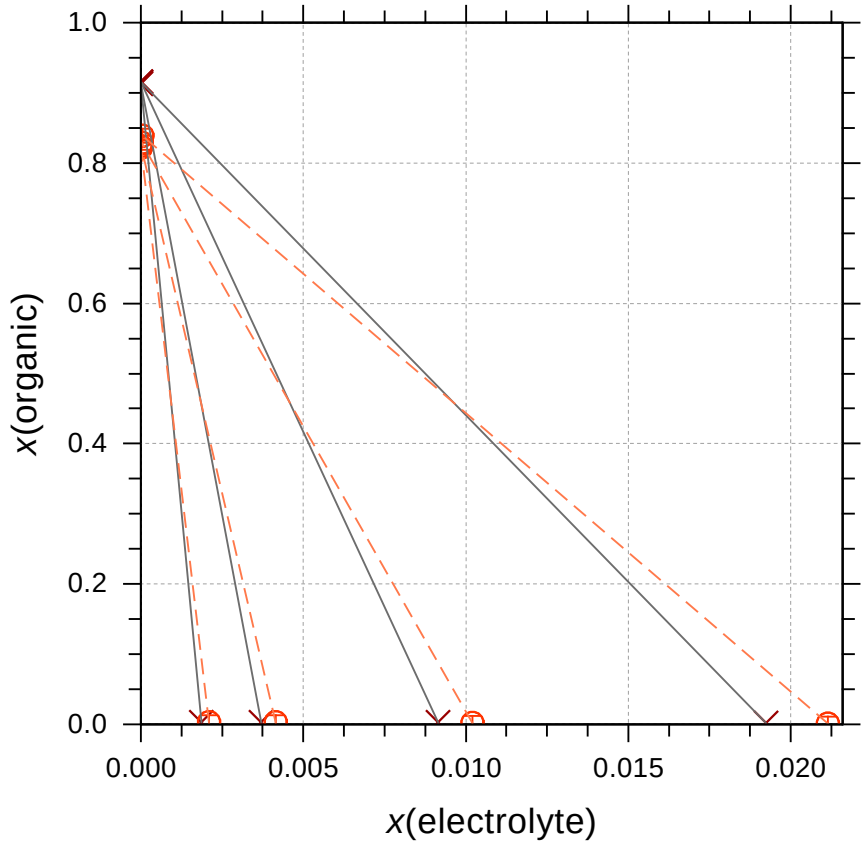
fval(0353) = 2.4589E-01

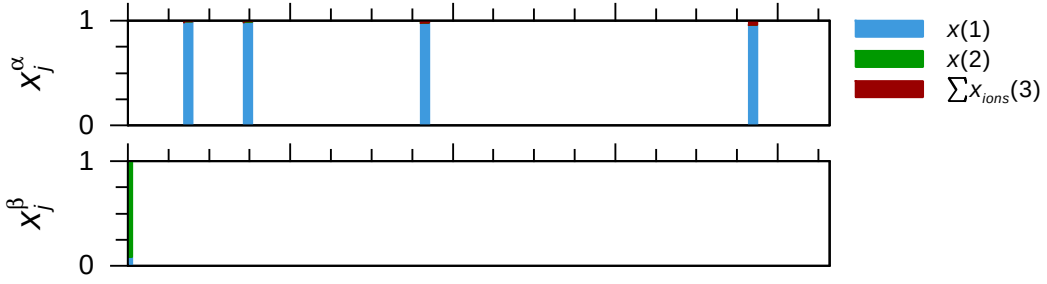
rel. contribution = 0.1169 %

Fig. S0324a (AIOMFAC_output_0353)

H_2O (1) + 4-Methyl-2-pentanone (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl+4-Methyl-2-pentanone+Water_LLE_Schunk

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0353) = 1.000

dataset contribution to F_{obj}:

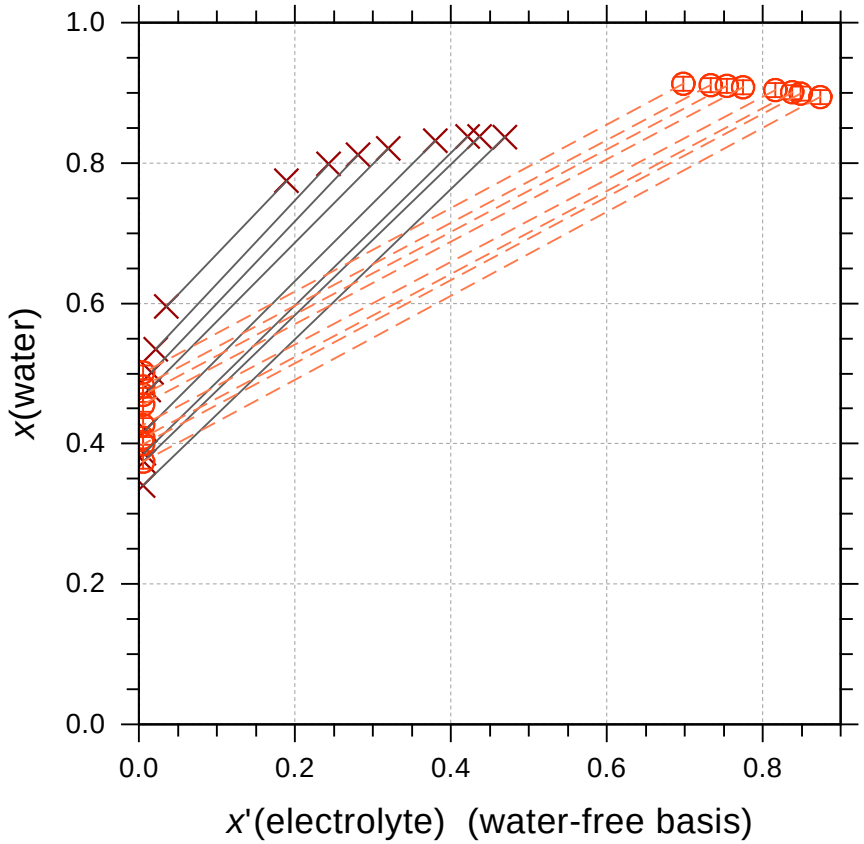
fval(0353) = 2.4589E-01

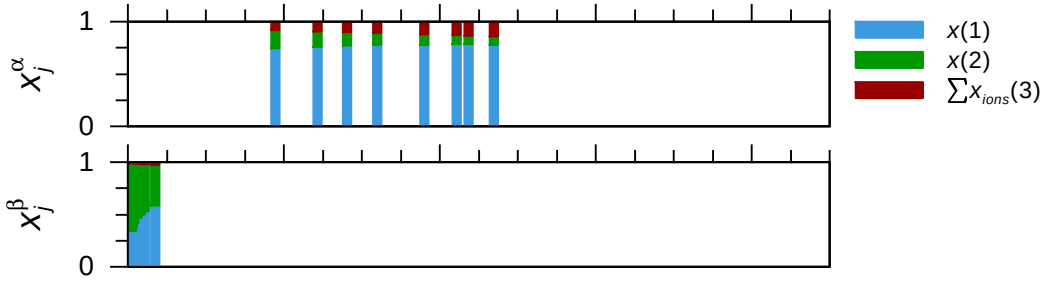
rel. contribution = 0.1169 %

Fig. S0325 (AIOMFAC_output_0392)

H_2O (1) + Acetone (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl+Acetone+Water_LLE_Marcilla

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0392) = 1.000

dataset contribution to F_{obj}:

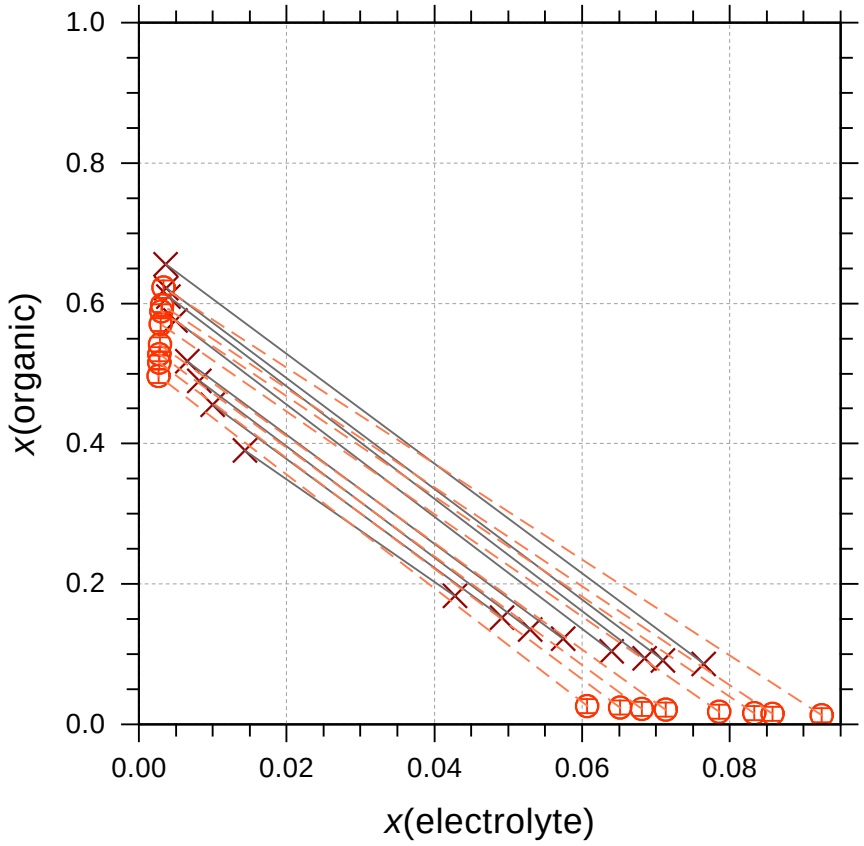
fval(0392) = 6.6011E-01

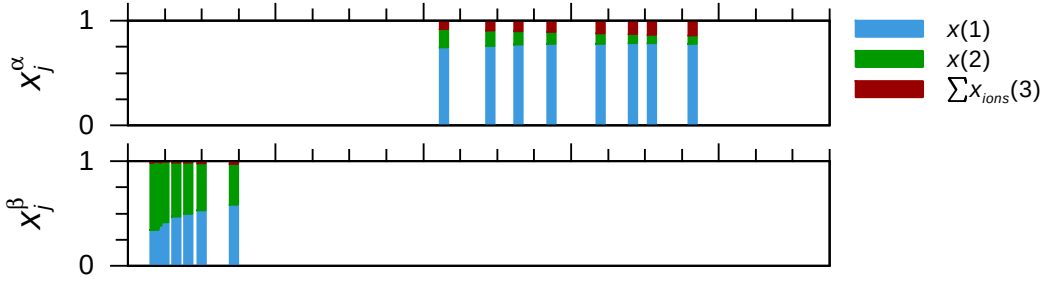
rel. contribution = 0.3139 %

Fig. S0325a (AIOMFAC_output_0392)

H_2O (1) + Acetone (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl+Acetone+Water_LLE_Marcilla

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

$w^{init}(0392)$ = 1.000

dataset contribution to F_{obj}:

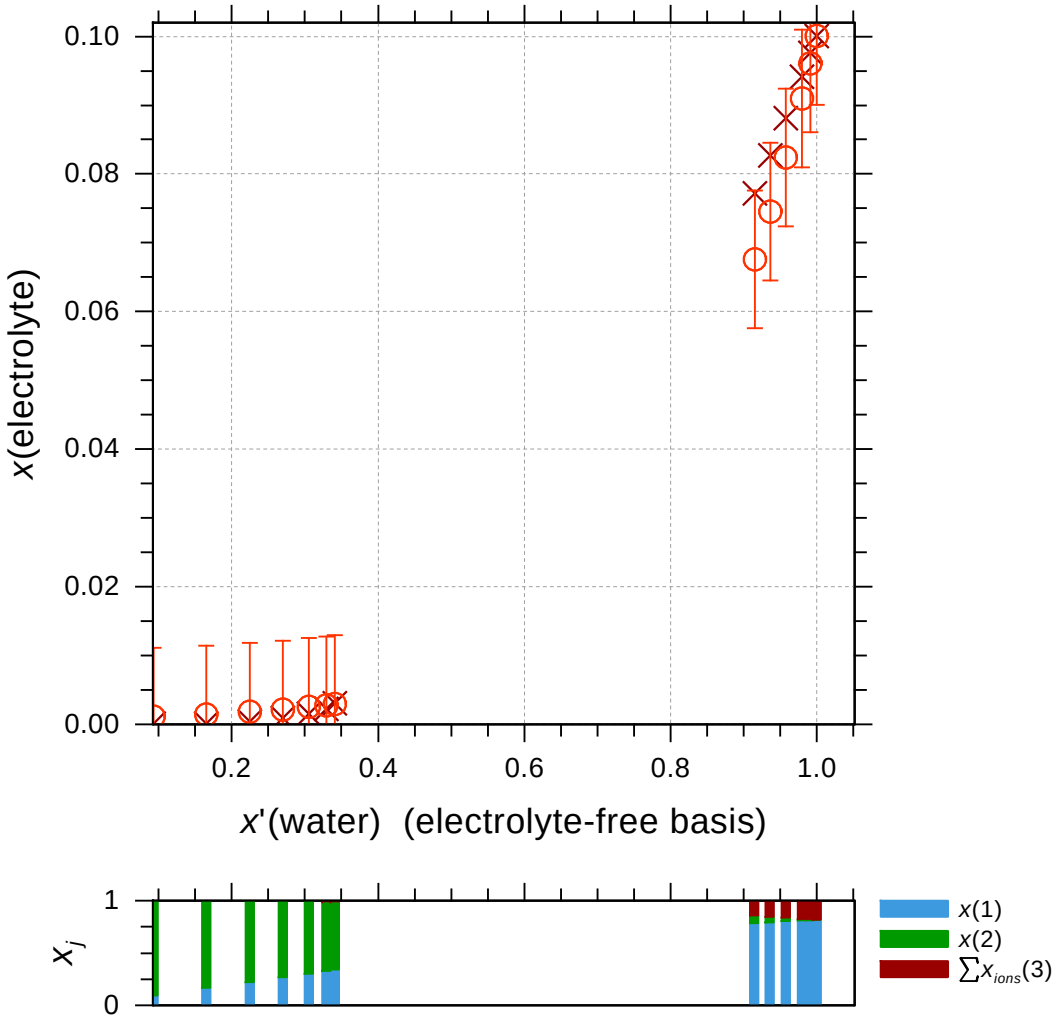
fval(0392) = 6.6011E-01

rel. contribution = 0.3139 %

Fig. S0326 (AIOMFAC_output_0393)

H_2O (1) + Acetone (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:
$w^{init}(0393)$ = 1.000
dataset contribution to F_{obj}:
fval(0393) = 7.1958E-02
rel. contribution = 0.0342 %

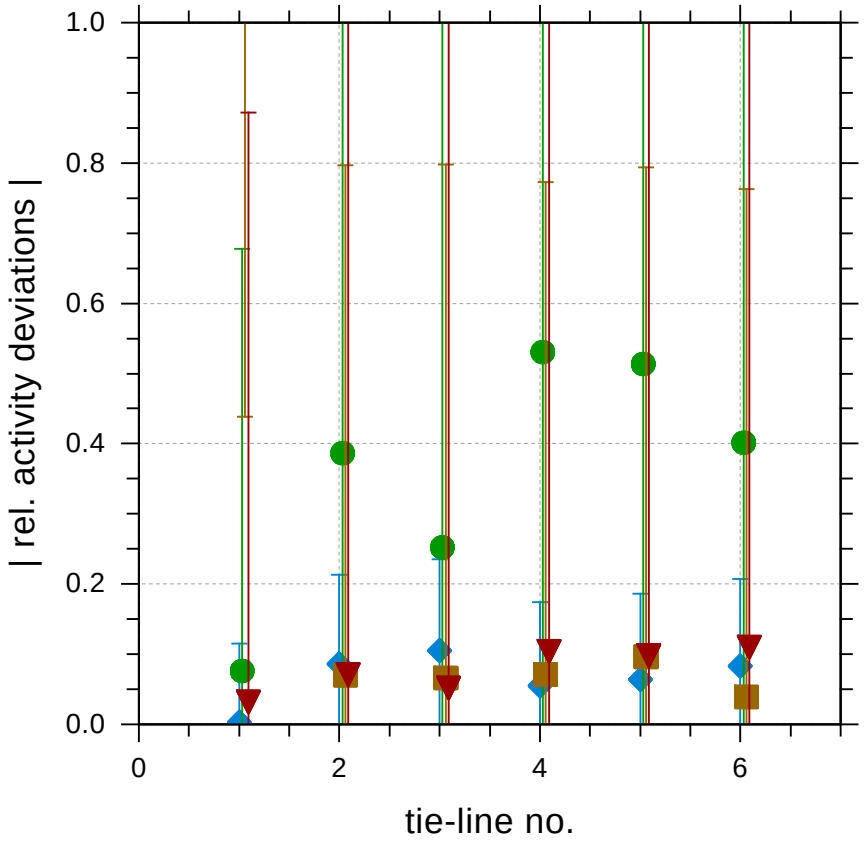
Fig. S0327 (AIOMFAC_output_0920)

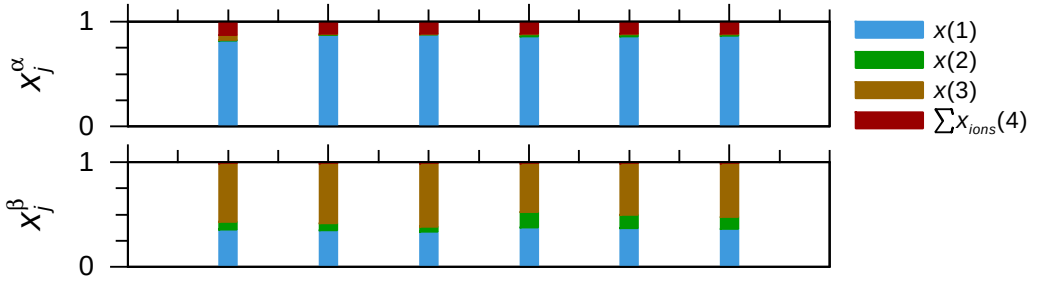
H_2O (1) + Acetone (2) + 1-Butanol (3) + NaCl (4)

Temperature: 293 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)





initial weighting of dataset:
$w^{init}(0920)$ = 0.800
dataset contribution to F_{obj}:
fval(0920) = 1.3970E+00
rel. contribution = 0.6643 %

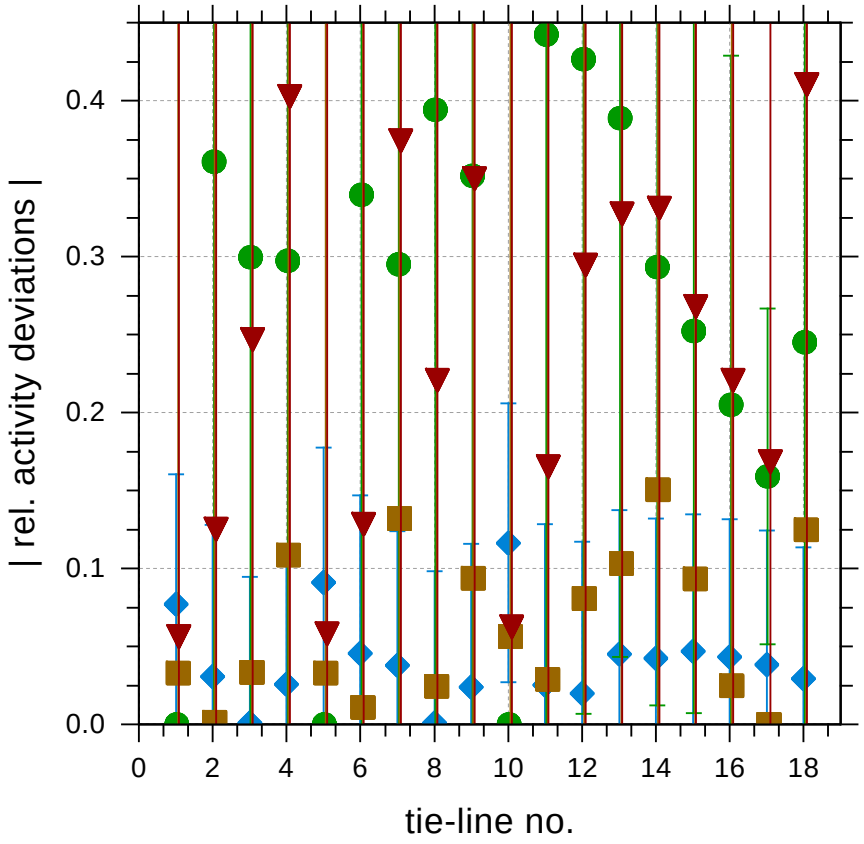
Fig. S0328 (AIOMFAC_output_0921)

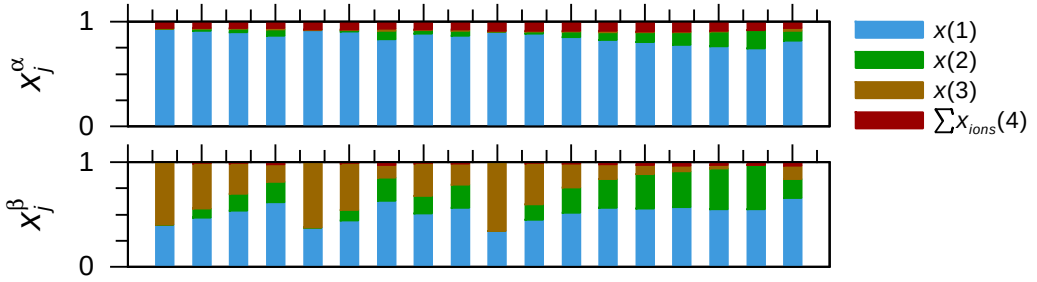
H_2O (1) + Acetone (2) + 1-Butanol (3) + NaCl (4)

Temperature: 298 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



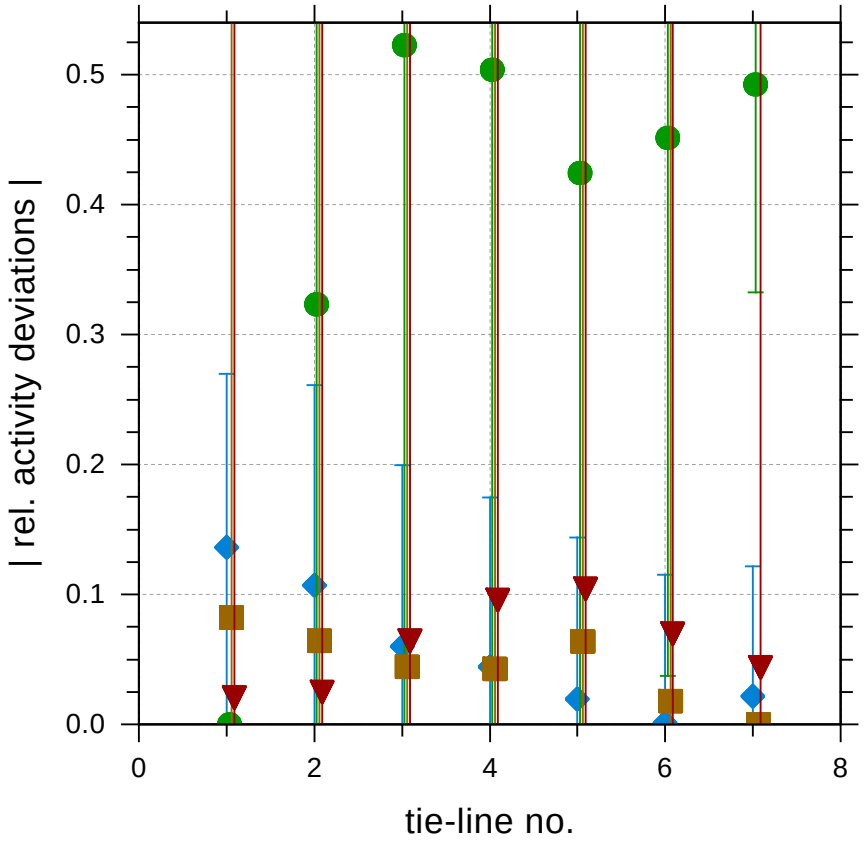


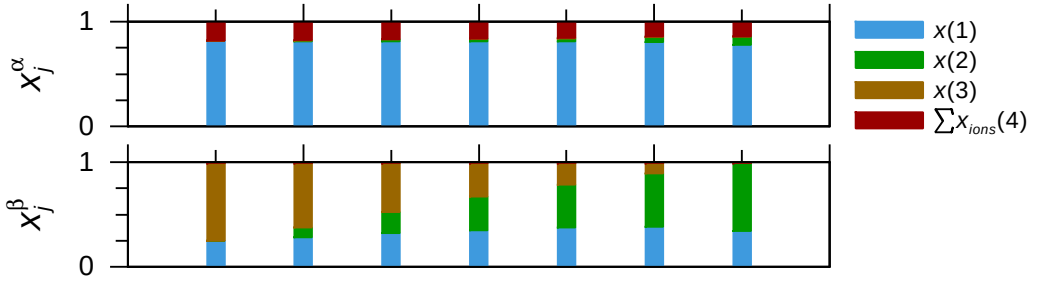
initial weighting of dataset:
$w^{init}(0921)$ = 0.800
dataset contribution to F_{obj}:
fval(0921) = 6.6134E-01
rel. contribution = 0.3145 %

Fig. S0329 (AIOMFAC_output_0922)

H_2O (1) + Acetone (2) + 1-Butanol (3) + NaCl (4)

Temperature: 298 K



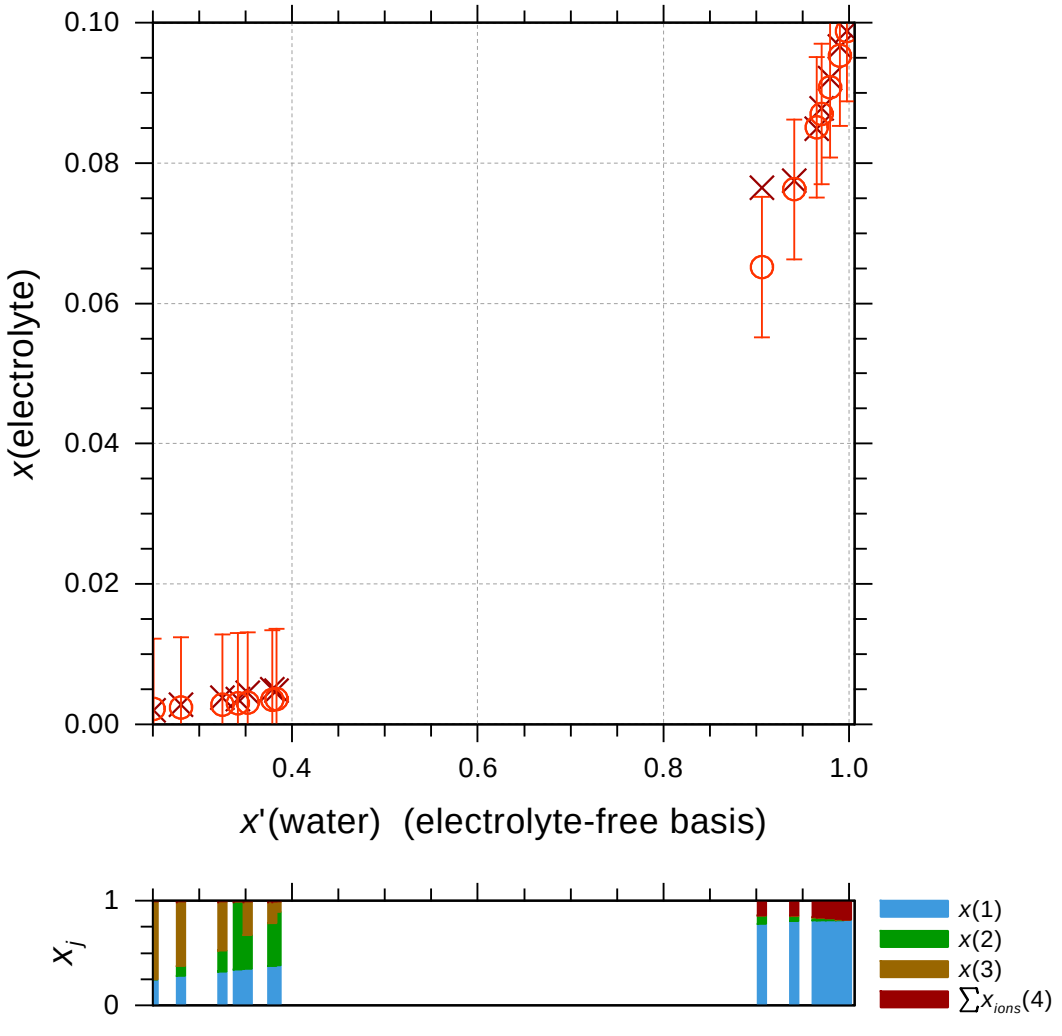


initial weighting of dataset:
$w^{init}(0922)$ = 0.800
dataset contribution to F_{obj}:
fval(0922) = 7.6876E-01
rel. contribution = 0.3656 %

Fig. S0330 (AIOMFAC_output_0923)

H_2O (1) + Acetone (2) + 1-Butanol (3) + NaCl (4)

Temperature: 298 K

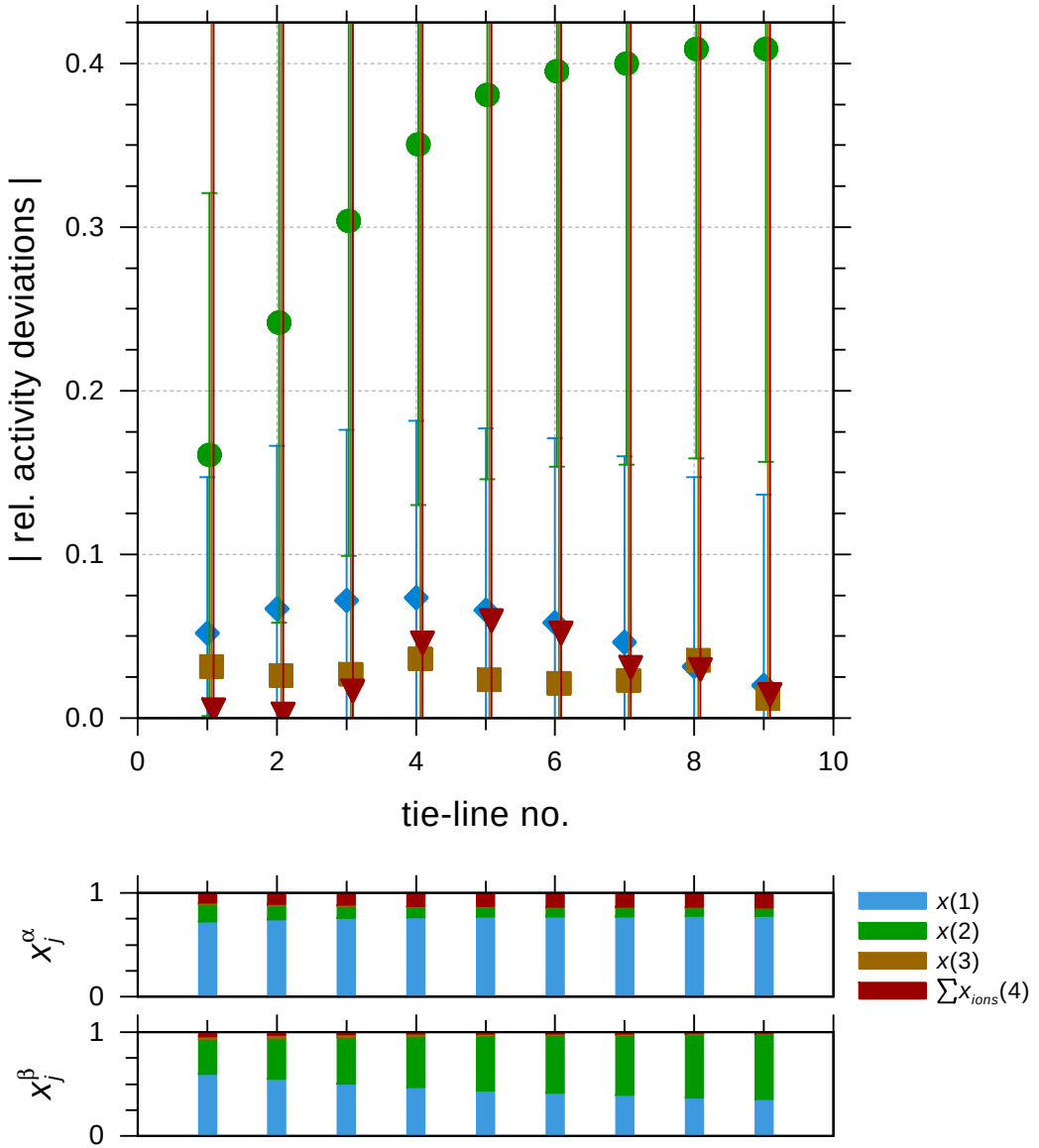


initial weighting of dataset:
$w^{init}(0923)$ = 1.000
dataset contribution to F_{obj}:
fval(0923) = 3.8740E-02
rel. contribution = 0.0184 %

Fig. S0331 (AIOMFAC_output_0927)

H_2O (1) + Acetone (2) + Ethanol (3) + NaCl (4)

Temperature: 298 K

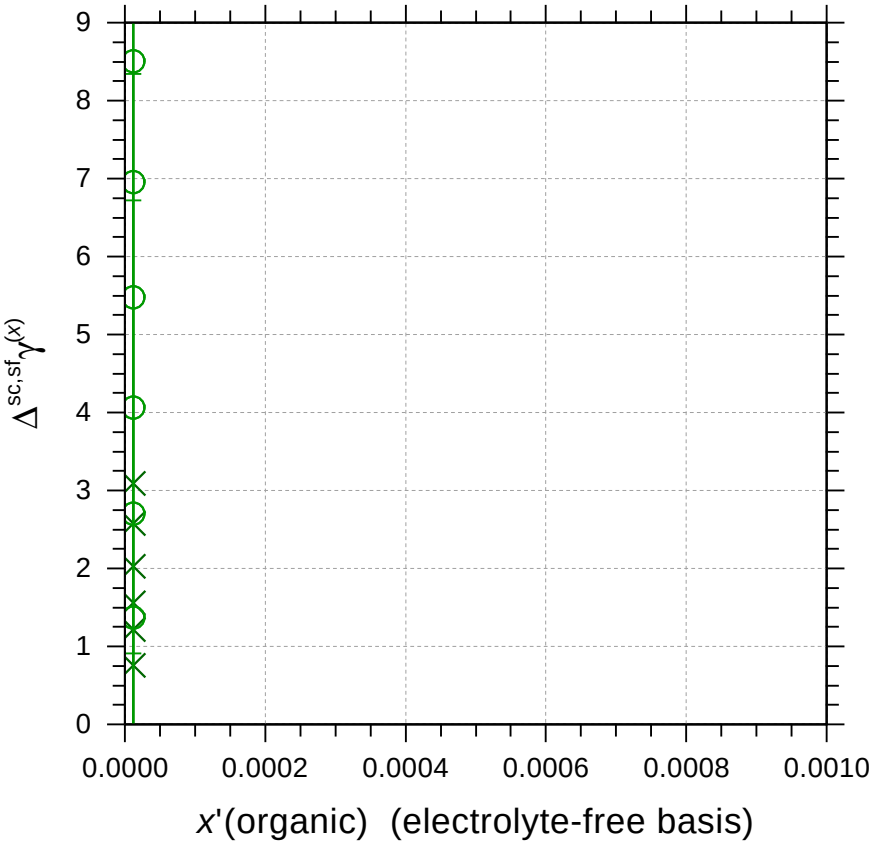


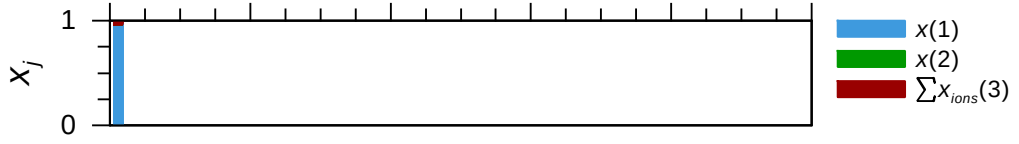
initial weighting of dataset:
$w^{init}(0927)$ = 0.800
dataset contribution to F_{obj}:
fval(0927) = 5.0746E-01
rel. contribution = 0.2413 %

Fig. S0332 (AIOMFAC_output_0984)

H_2O (1) + Acetone (2) + NaCl (3)

Temperature: 313 K



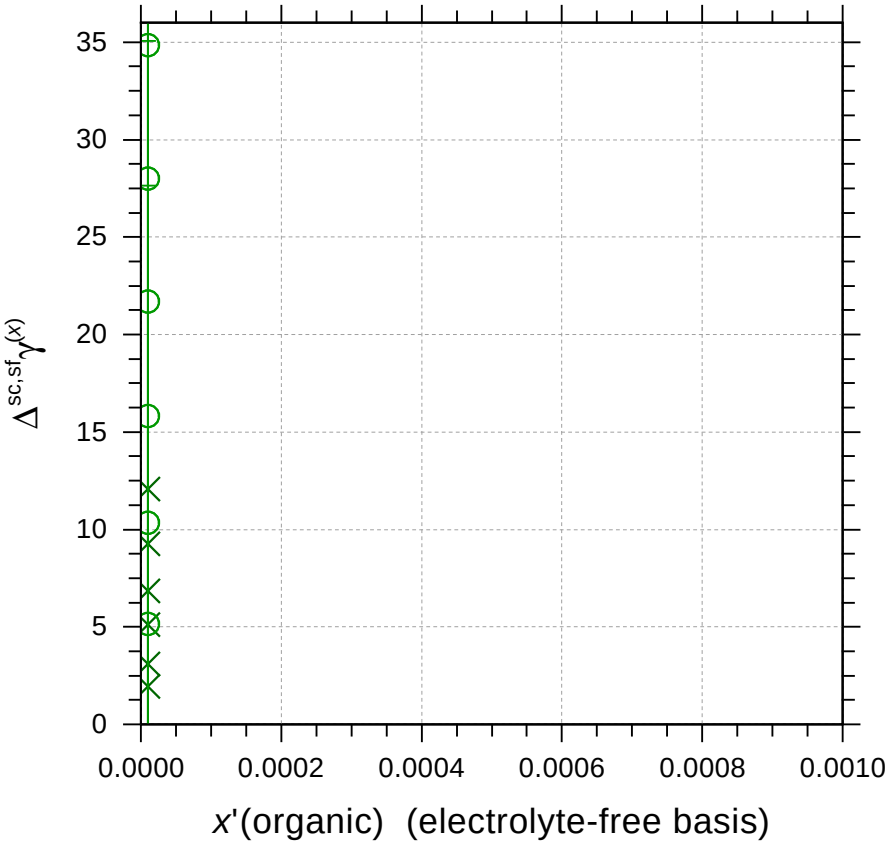


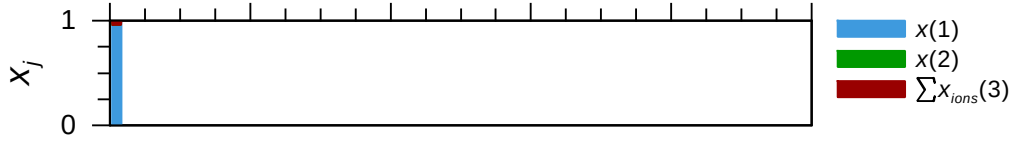
initial weighting of dataset:
w^{init}(0984) = 0.100
dataset contribution to F_{obj}:
fval(0984) = 9.2938E-02
rel. contribution = 0.0442 %

Fig. S0333 (AIOMFAC_output_0985)

H_2O (1) + 2-Butanone (2) + NaCl (3)

Temperature: 313 K



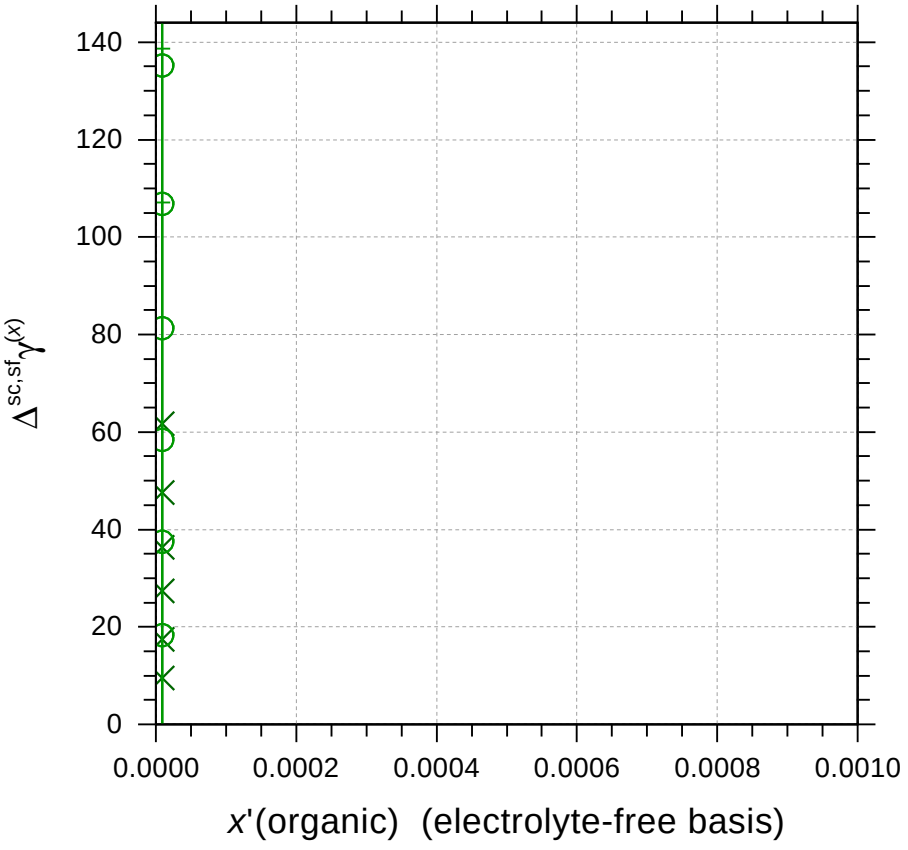


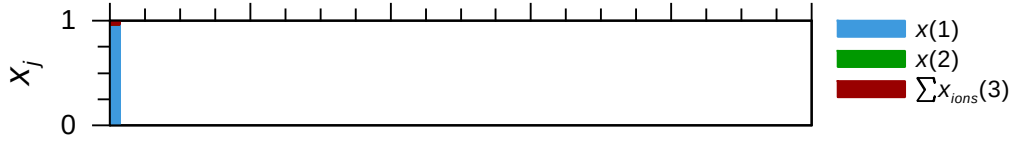
initial weighting of dataset:
$w^{init}(0985)$ = 0.100
dataset contribution to F_{obj}:
fval(0985) = 7.0980E-02
rel. contribution = 0.0338 %

Fig. S0334 (AIOMFAC_output_0986)

H_2O (1) + 2-Pentanone (2) + NaCl (3)

Temperature: 313 K



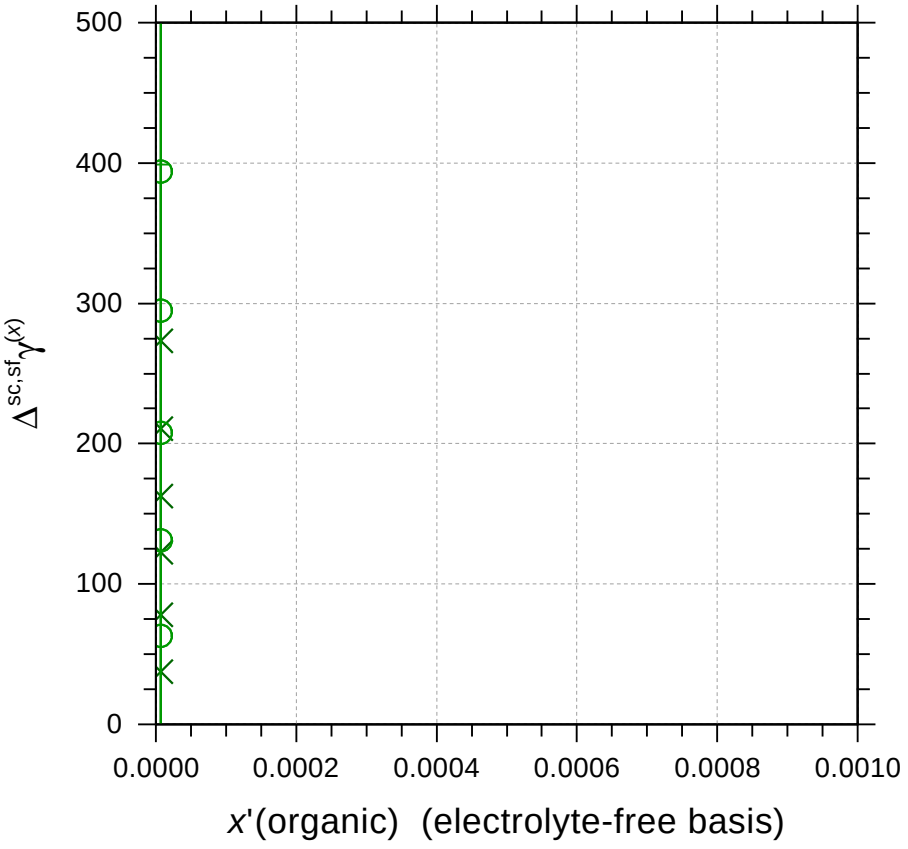


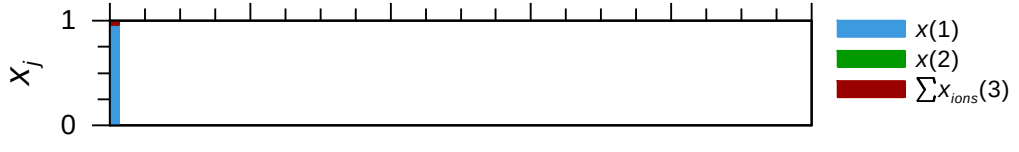
initial weighting of dataset:
$w^{init}(0986)$ = 0.100
dataset contribution to F_{obj}:
fval(0986) = 3.3257E-02
rel. contribution = 0.0158 %

Fig. S0335 (AIOMFAC_output_0987)

H_2O (1) + 2-Hexanone (2) + NaCl (3)

Temperature: 313 K



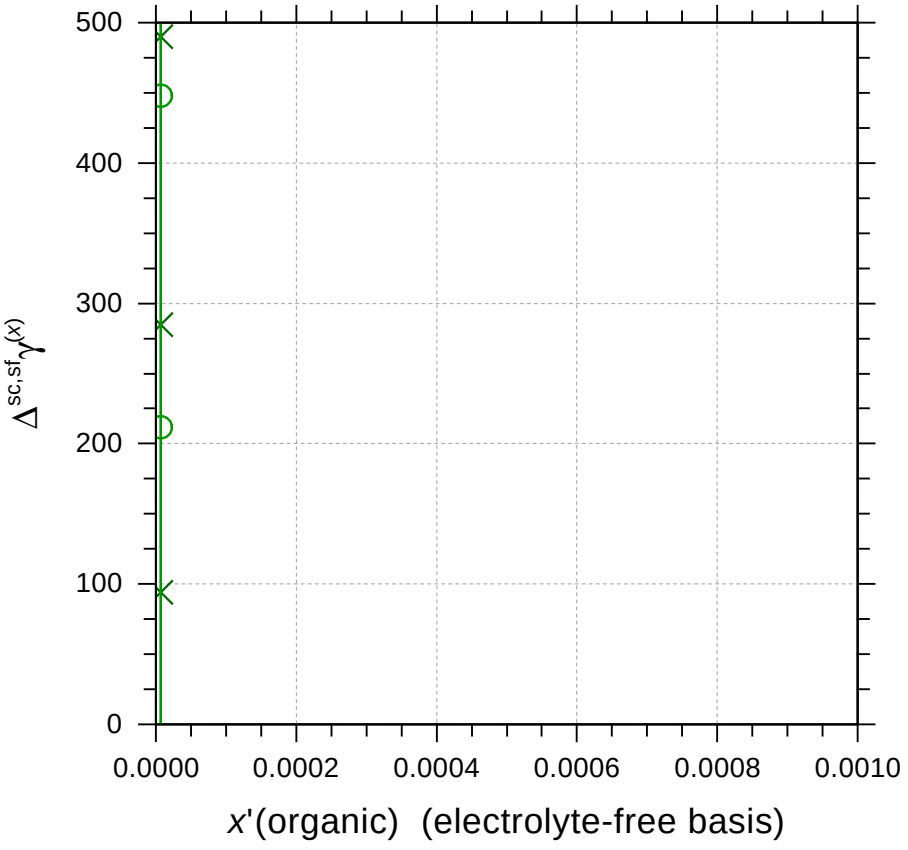


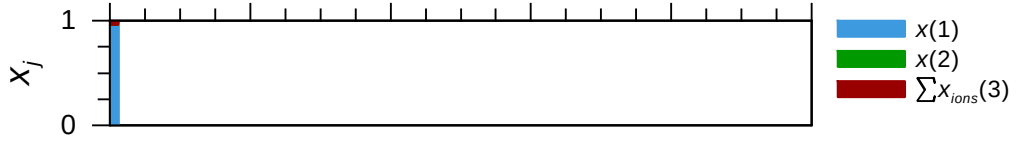
initial weighting of dataset:
$w^{init}(0987)$ = 0.100
dataset contribution to F_{obj}:
fval(0987) = 1.6404E-02
rel. contribution = 0.0078 %

Fig. S0336 (AIOMFAC_output_0988)

H_2O (1) + 2-Heptanone (2) + NaCl (3)

Temperature: 313 K





left y-axis:

× NaCl+2-Heptanone+Water_VLE_Falabella (EXP, org.)

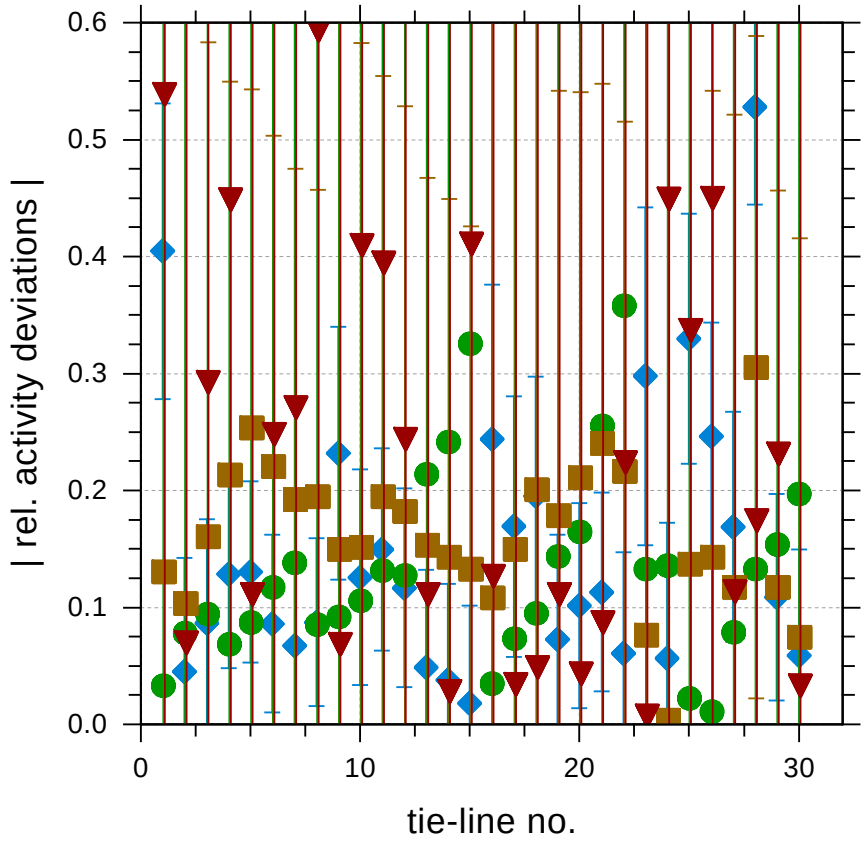
○ AIOMFAC $\Delta^{sc,sf}\gamma^{(x)}_{org.}$

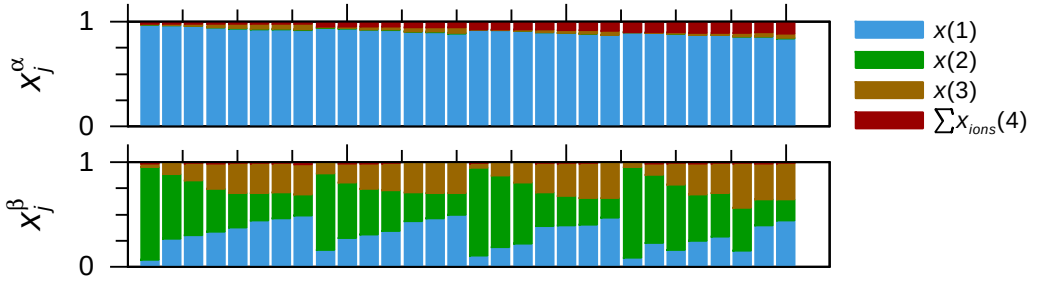
initial weighting of dataset:
w^{init}(0988) = 0.100
dataset contribution to F_{obj}:
fval(0988) = 8.8667E-03
rel. contribution = 0.0042 %

Fig. S0337 (AIOMFAC_output_0303)

H_2O (1) + 4-Methyl-2-pentanone (2) + Propanoic_acid (3) + $NaNO_3$ (4)

Temperature: 308 K





left y-axis:

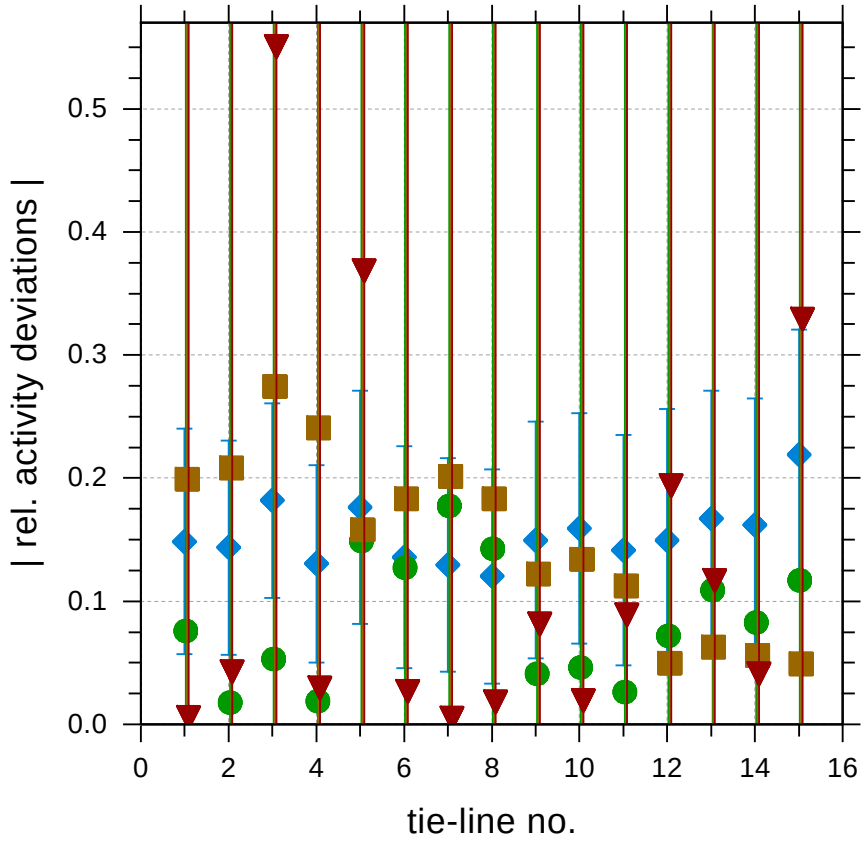
- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

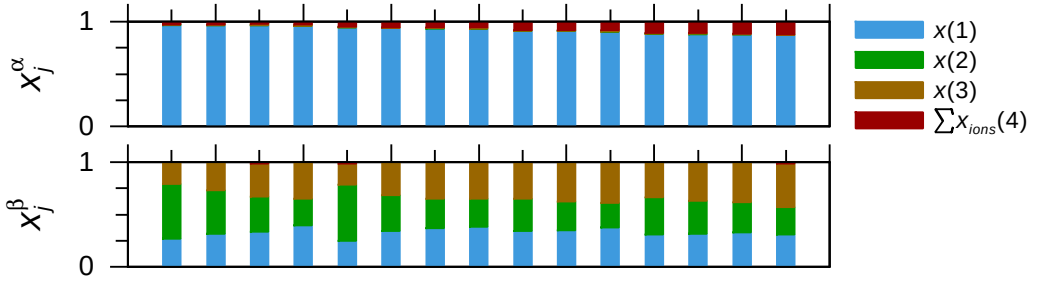
initial weighting of dataset:
w^{init}(0303) = 1.000
dataset contribution to F_{obj}:
fval(0303) = 8.3947E-01
rel. contribution = 0.3992 %

Fig. S0338 (AIOMFAC_output_0307)

H_2O (1) + 4-Methyl-2-pentanone (2) + Butyric_acid (3) + $NaNO_3$ (4)

Temperature: 308 K





left y-axis:

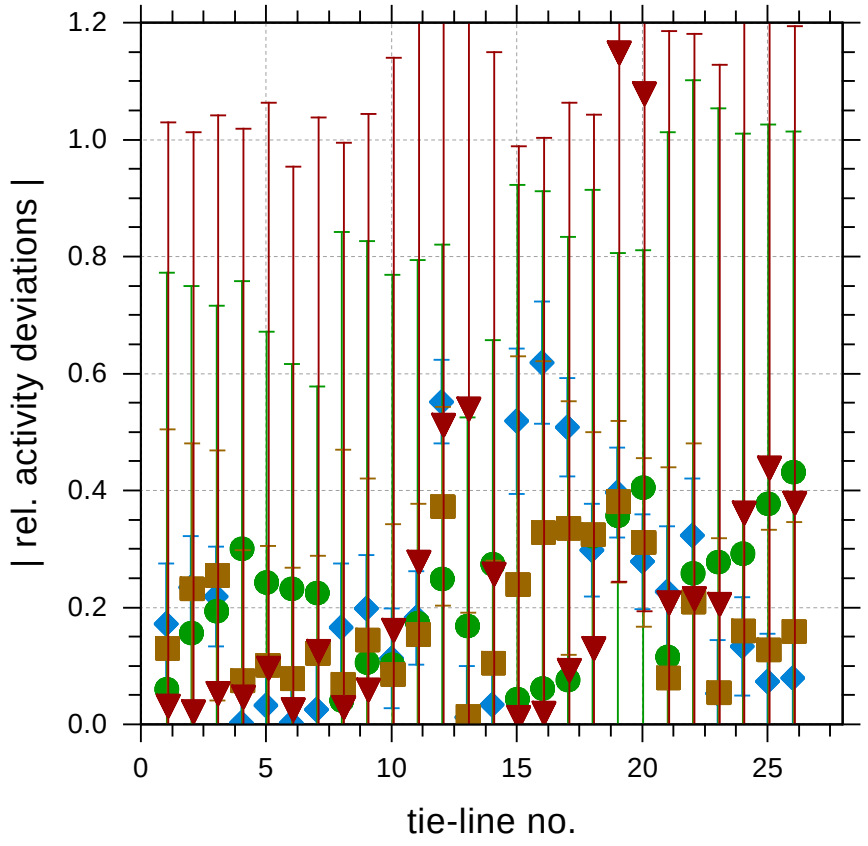
- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

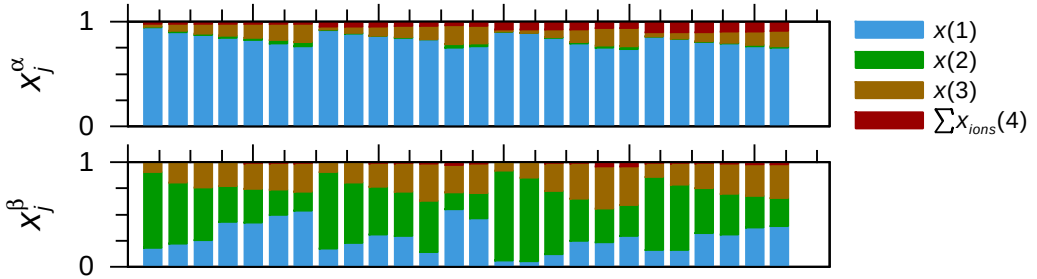
initial weighting of dataset:
w^{init}(0307) = 1.000
dataset contribution to F_{obj}:
fval(0307) = 5.1094E-01
rel. contribution = 0.2430 %

Fig. S0339 (AIOMFAC_output_0314)

H_2O (1) + 4-Methyl-2-pentanone (2) + Acetic_acid (3) + $NaNO_3$ (4)

Temperature: 308 K





left y-axis:

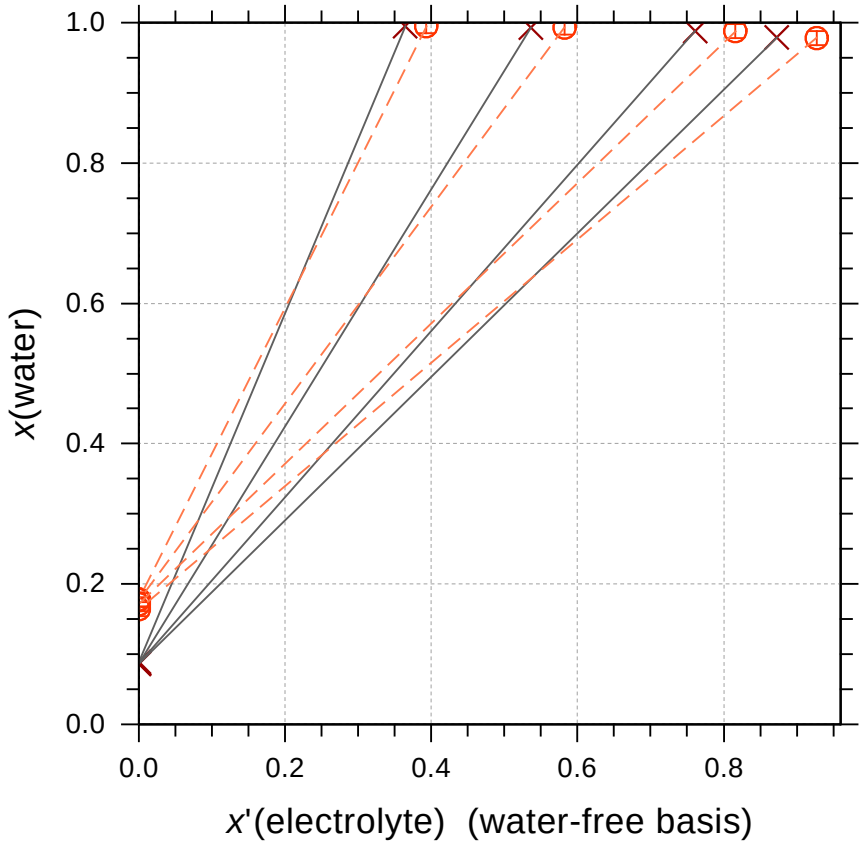
- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

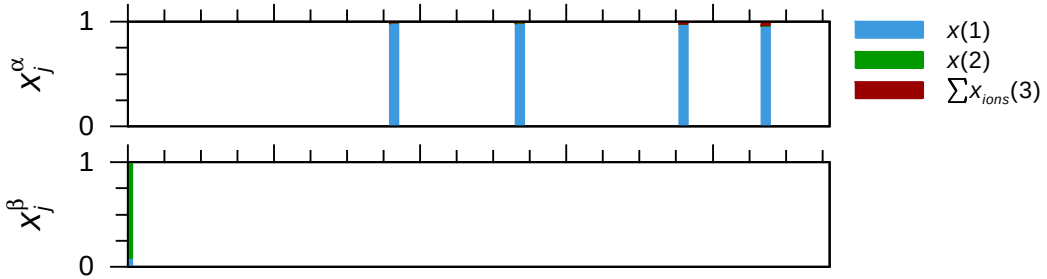
initial weighting of dataset:
w^{init}(0314) = 1.000
dataset contribution to F_{obj}:
fval(0314) = 1.6289E+00
rel. contribution = 0.7746 %

Fig. S0340 (AIOMFAC_output_0354)

H_2O (1) + 4-Methyl-2-pentanone (2) + $NaNO_3$ (3)

Temperature: 298 K





left y-axis:

× NaNO3+4-Methyl-2-pentanone+Water_LLE_Schunk

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0354) = 1.000

dataset contribution to F_{obj}:

fval(0354) = 2.3801E-01

rel. contribution = 0.1132 %

Fig. S0340a (AIOMFAC_output_0354)

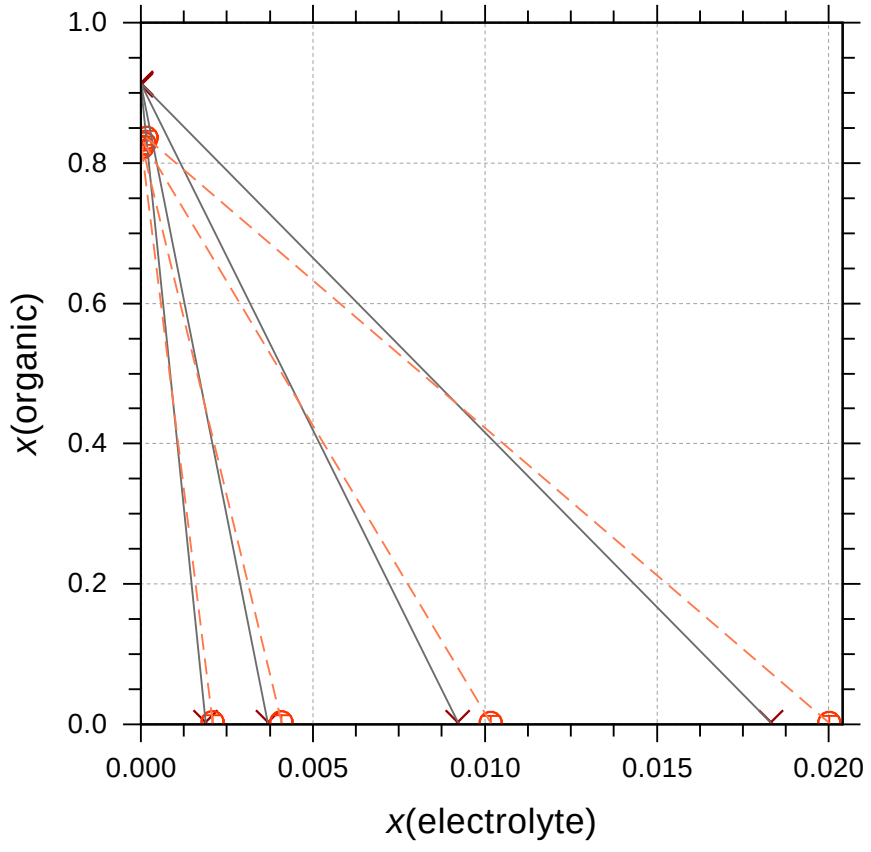
H_2O (1) + 4-Methyl-2-pentanone (2) + $NaNO_3$ (3)

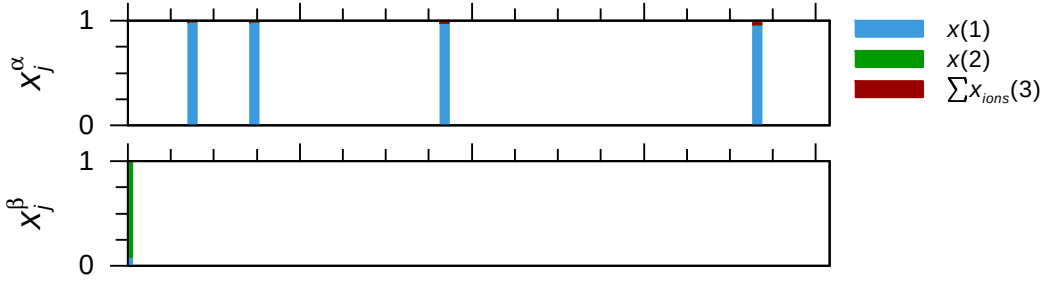
Temperature: 298 K

left y-axis:

× NaNO3+4-Methyl-2-pentanone+Water_LLE_Schunk

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0354)$ = 1.000

dataset contribution to F_{obj}:

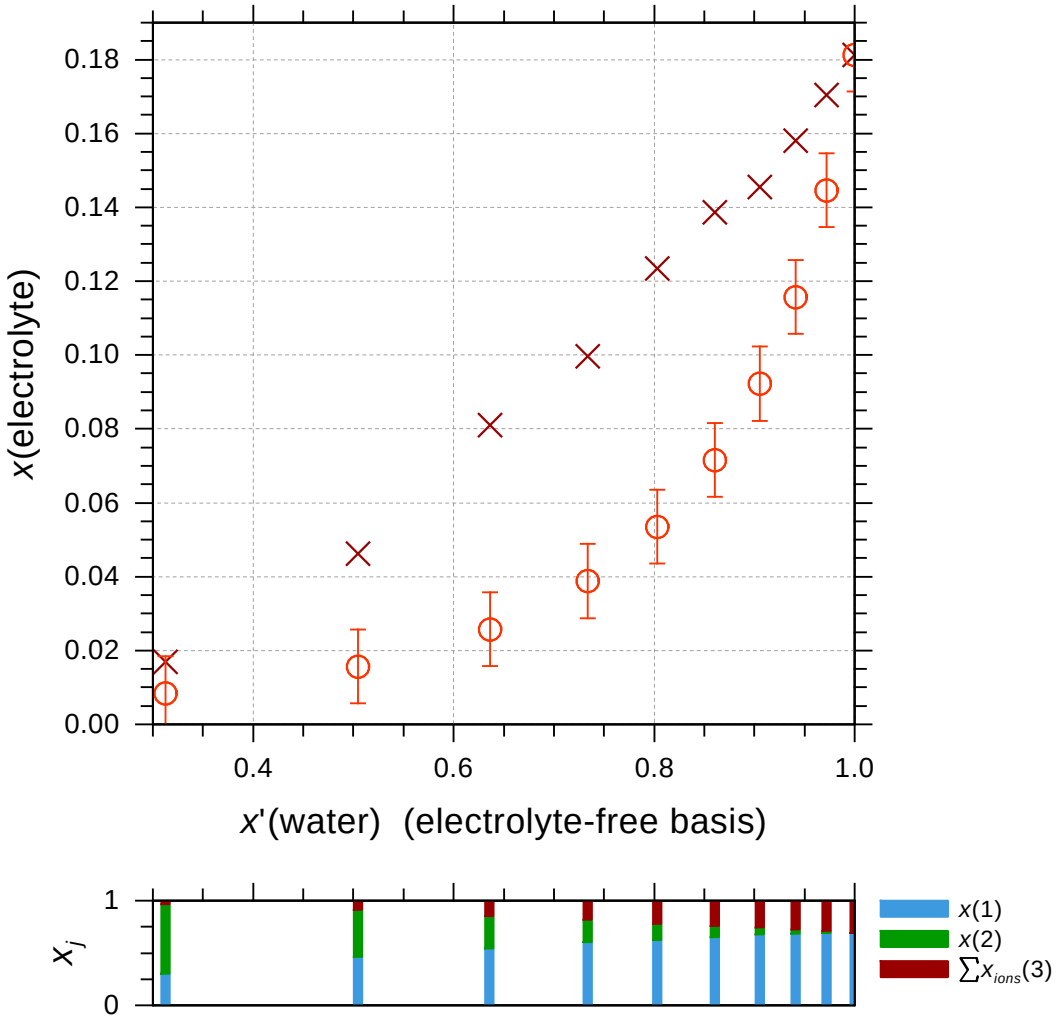
fval(0354) = 2.3801E-01

rel. contribution = 0.1132 %

Fig. S0341 (AIOMFAC_output_0944)

H_2O (1) + Acetone (2) + $NaNO_3$ (3)

Temperature: 313 K

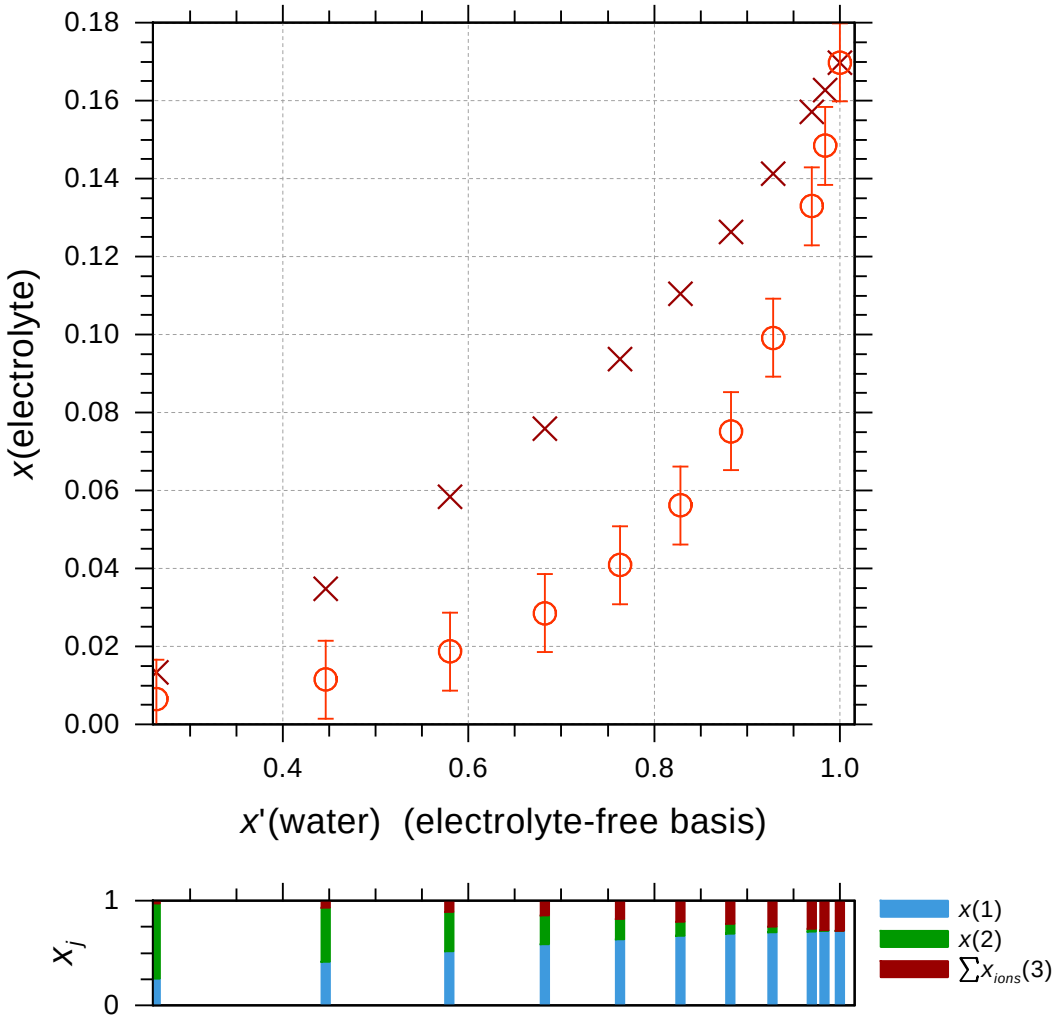


initial weighting of dataset:
$w^{init}(0944)$ = 0.500
dataset contribution to F_{obj}:
fval(0944) = 9.0189E-01
rel. contribution = 0.4289 %

Fig. S0342 (AIOMFAC_output_0945)

H_2O (1) + Acetone (2) + $NaNO_3$ (3)

Temperature: 303 K

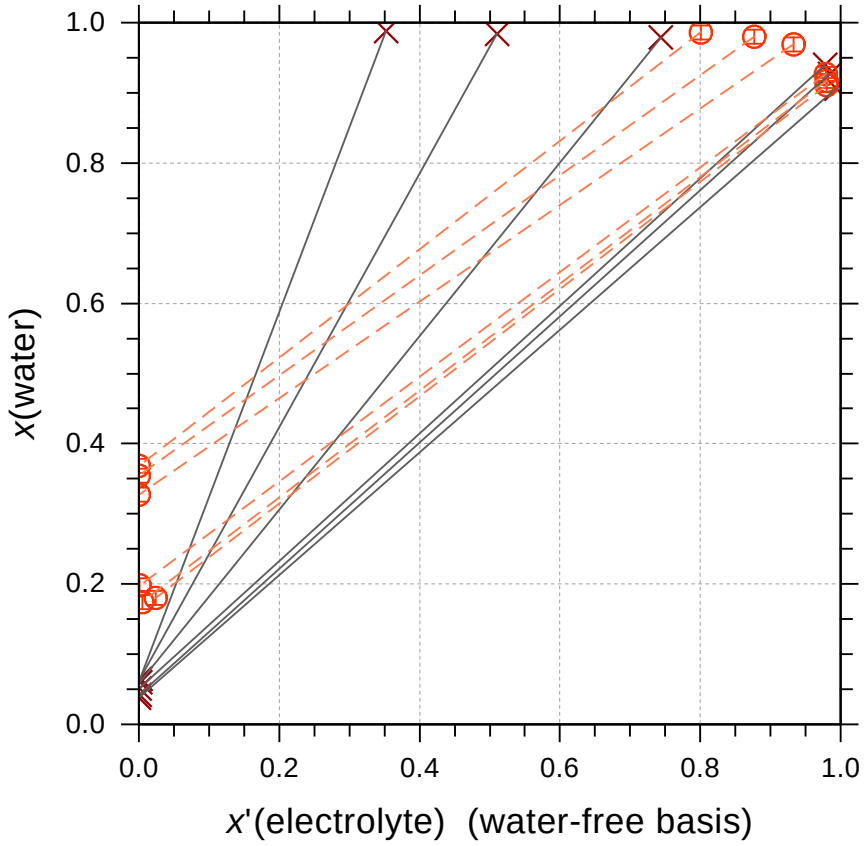


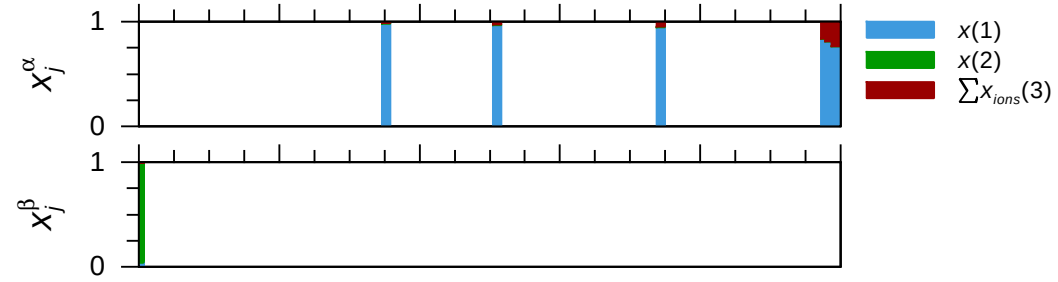
initial weighting of dataset:
$w^{init}(0945)$ = 0.500
dataset contribution to F_{obj}:
fval(0945) = 7.9045E-01
rel. contribution = 0.3759 %

Fig. S0343 (AIOMFAC_output_0367)

H_2O (1) + 2-Methoxy-2-methylpropane (2) + $CaCl_2$ (3)

Temperature: 298 K





left y-axis:

× CaCl2+2-Methoxy-2-methylpropane+Water_LLE_Salabat

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0367) = 1.000

dataset contribution to F_{obj}:

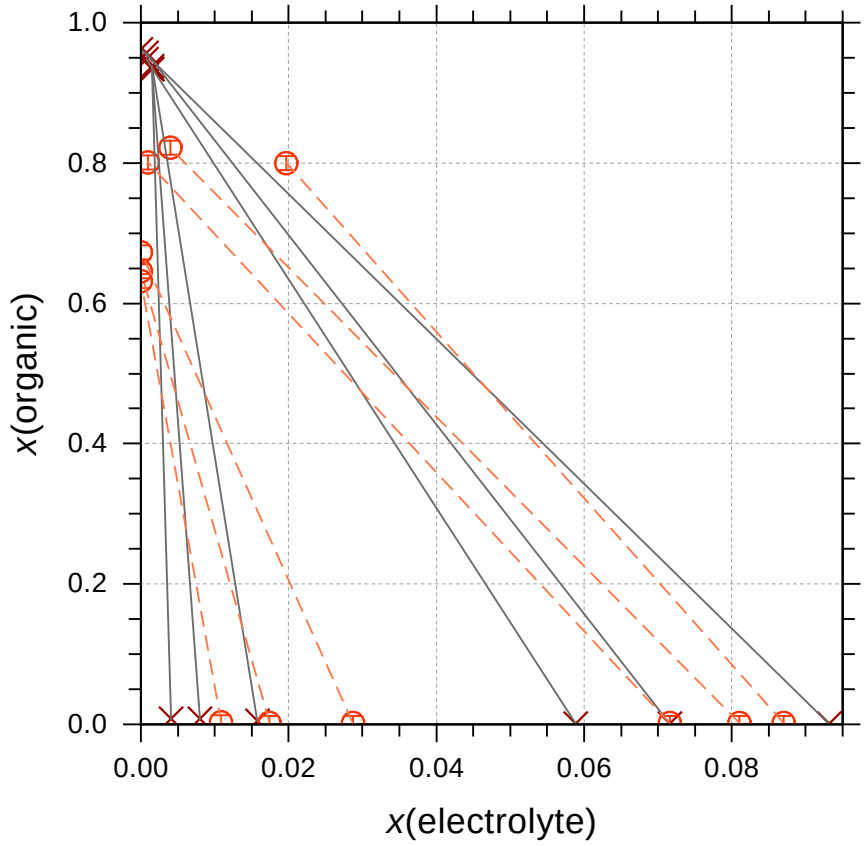
fval(0367) = 2.3643E+00

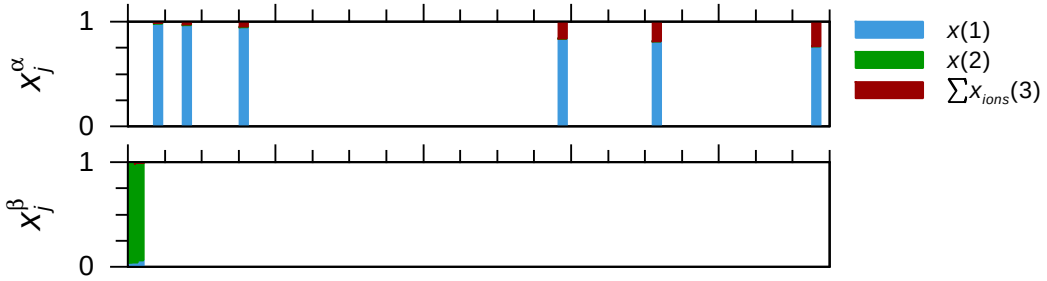
rel. contribution = 1.1243 %

Fig. S0343a (AIOMFAC_output_0367)

H_2O (1) + 2-Methoxy-2-methylpropane (2) + $CaCl_2$ (3)

Temperature: 298 K





left y-axis:

× CaCl2+2-Methoxy-2-methylpropane+Water_LLE_Salabat

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0367) = 1.000

dataset contribution to F_{obj}:

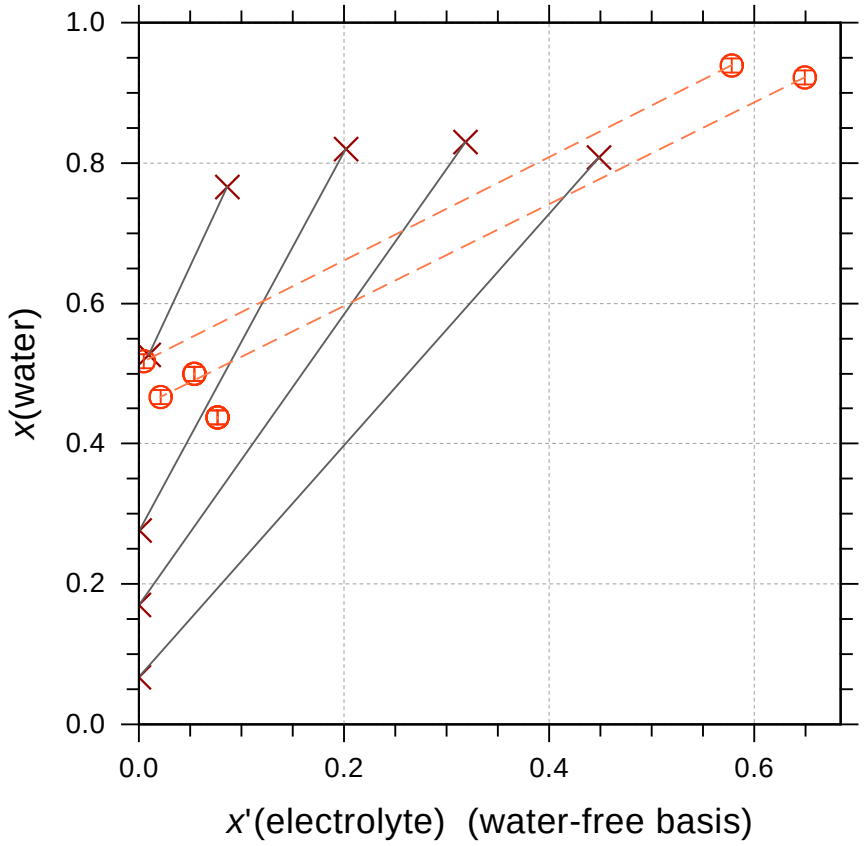
fval(0367) = 2.3643E+00

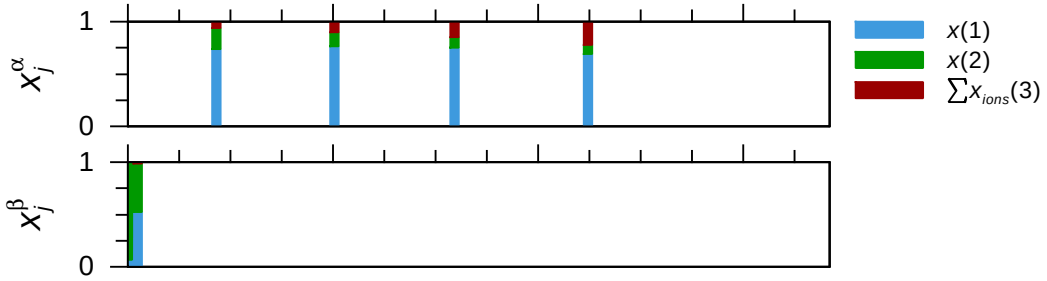
rel. contribution = 1.1243 %

Fig. S0344 (AIOMFAC_output_0439)

H_2O (1) + 1,4-Dioxane (2) + $CaCl_2$ (3)

Temperature: 298 K





left y-axis:

× CaCl2+1,4-Dioxane+Water_LLE_Bogardus

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0439) = 1.000

dataset contribution to F_{obj}:

fval(0439) = 7.9498E-01

rel. contribution = 0.3780 %

Fig. S0344a (AIOMFAC_output_0439)

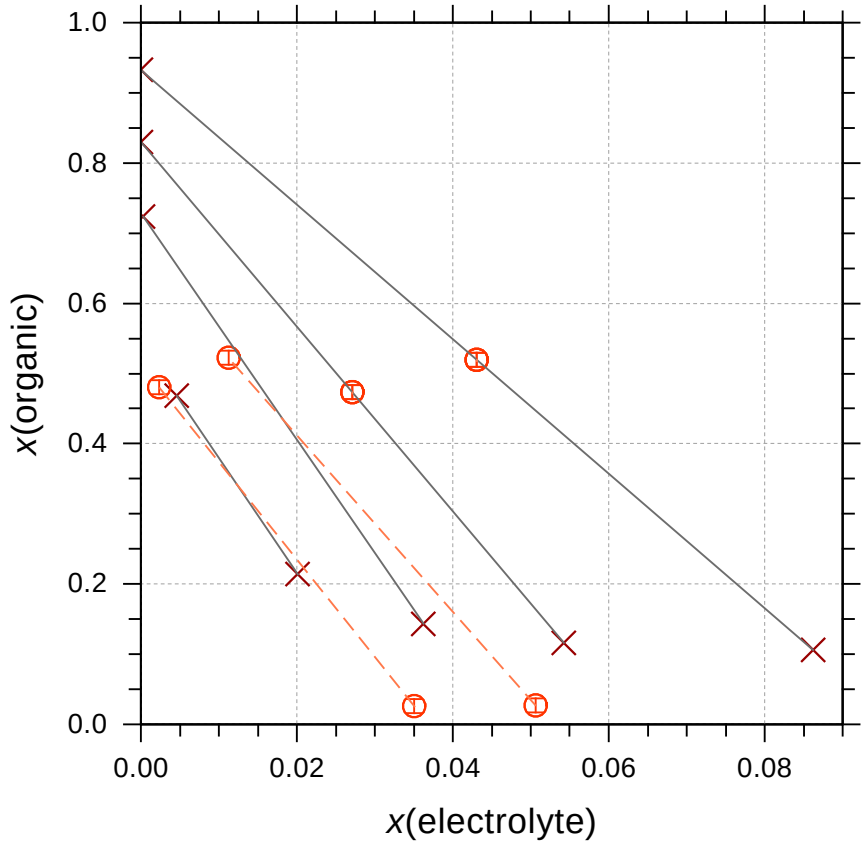
H_2O (1) + 1,4-Dioxane (2) + $CaCl_2$ (3)

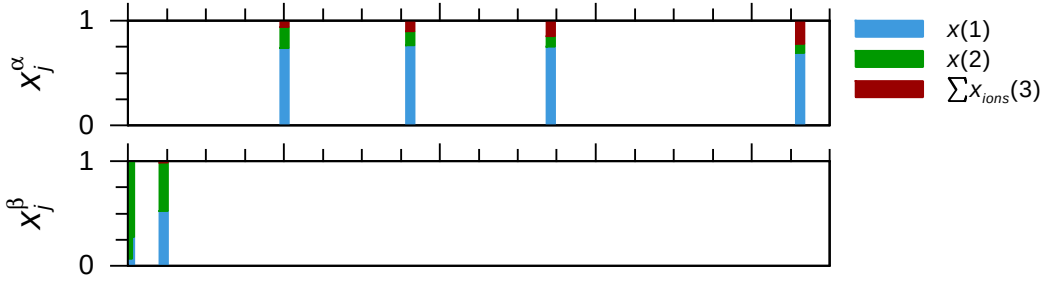
Temperature: 298 K

left y-axis:

× CaCl2+1,4-Dioxane+Water_LLE_Bogardus

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0439) = 1.000

dataset contribution to F_{obj}:

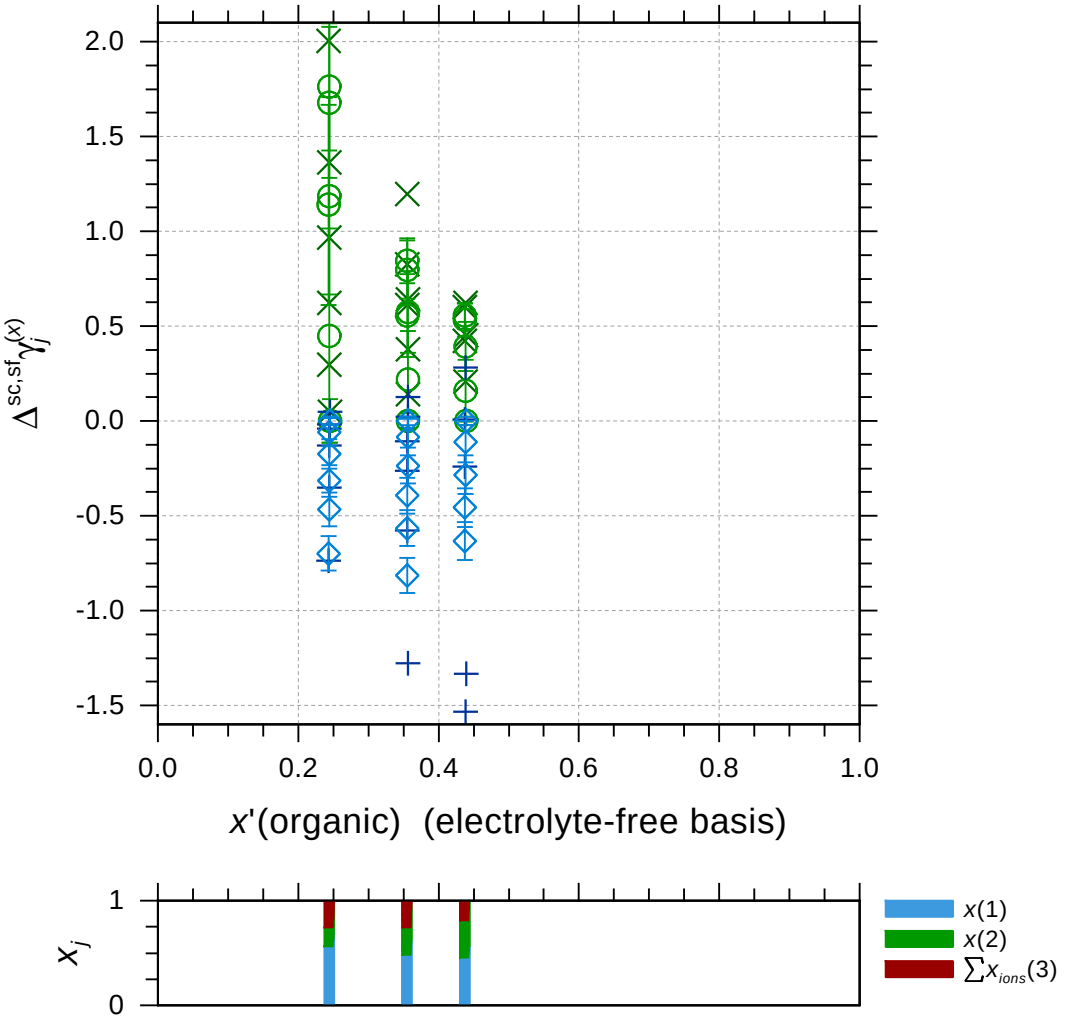
fval(0439) = 7.9498E-01

rel. contribution = 0.3780 %

Fig. S0345 (AIOMFAC_output_0931)

H_2O (1) + Tetrahydrofuran (2) + $CaCl_2$ (3)

Temperature range: 337 -- 338 K

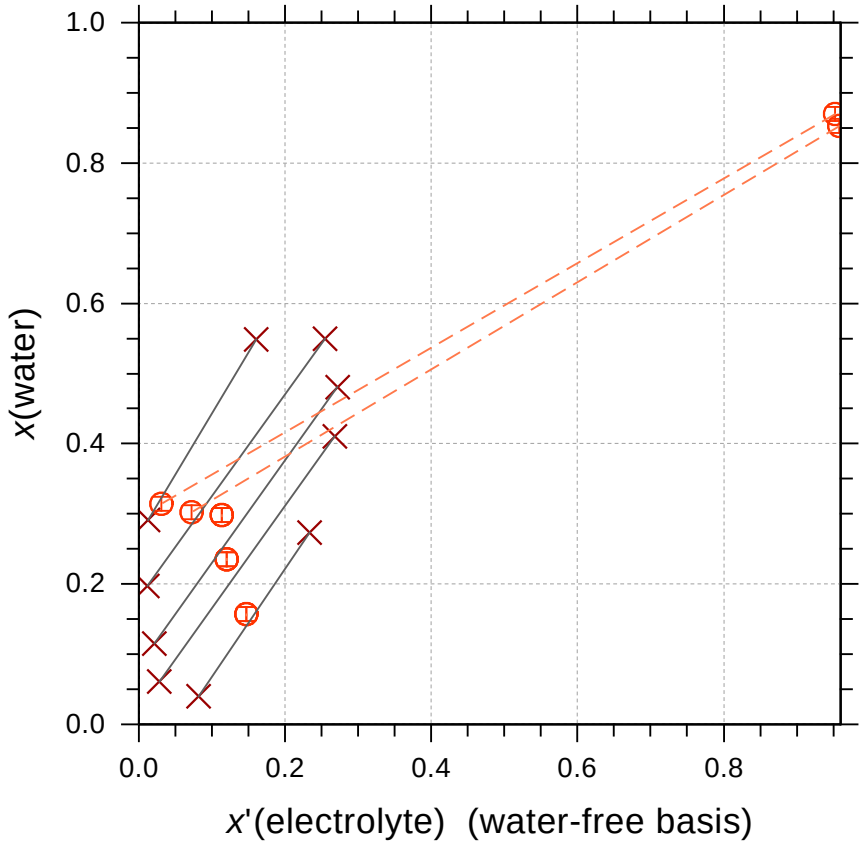


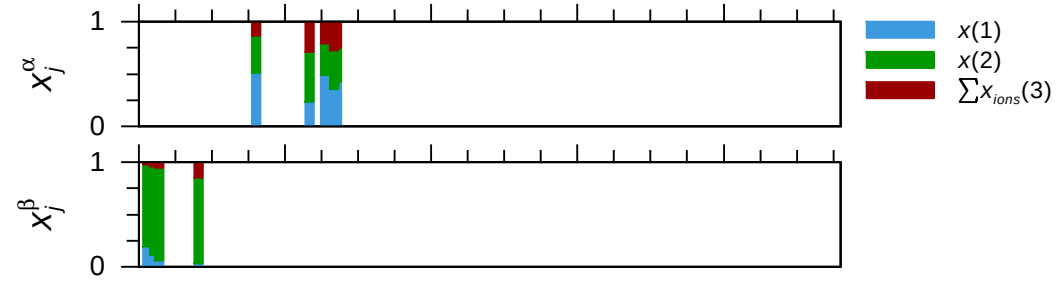
initial weighting of dataset:
w^{init}(0931) = 0.200
dataset contribution to F_{obj}:
fval(0931) = 2.6898E-01
rel. contribution = 0.1279 %

Fig. S0346 (AIOMFAC_output_0440)

H_2O (1) + 1,4-Dioxane (2) + HCl (3)

Temperature: 298 K





left y-axis:

× HCl+1,4-Dioxane+Water_LLE_Robinson

○ AIOMFAC calc. LLE composition

initial weighting of dataset:
w^{init}(0440) = 0.200
dataset contribution to F_{obj}:
fval(0440) = 1.4280E+00
rel. contribution = 0.6790 %

Fig. S0346a (AIOMFAC_output_0440)

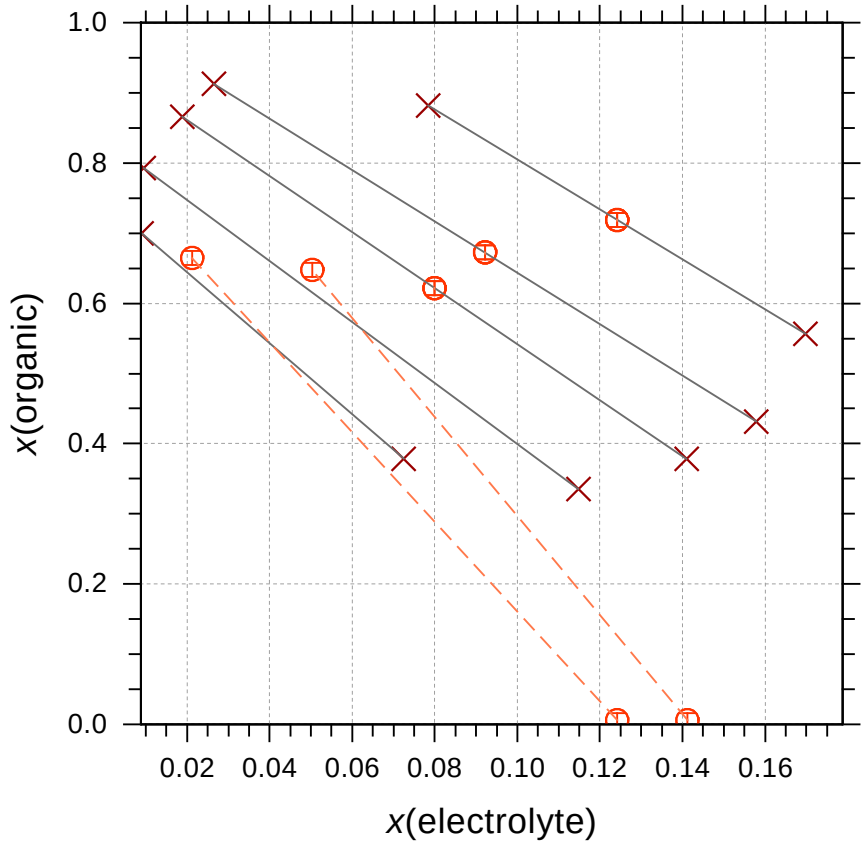
H_2O (1) + 1,4-Dioxane (2) + HCl (3)

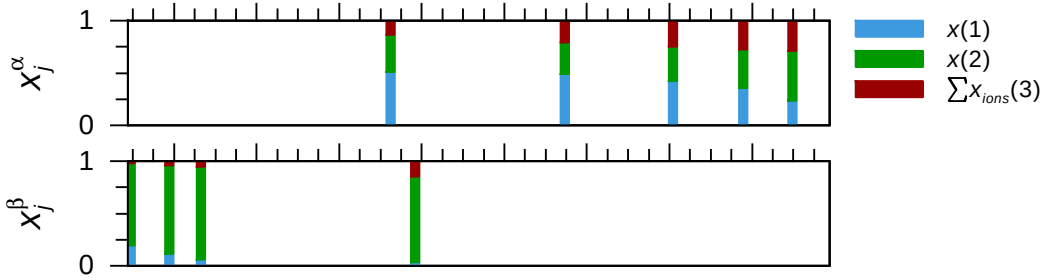
Temperature: 298 K

left y-axis:

× HCl+1,4-Dioxane+Water_LLE_Robinson

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0440) = 0.200

dataset contribution to F_{obj}:

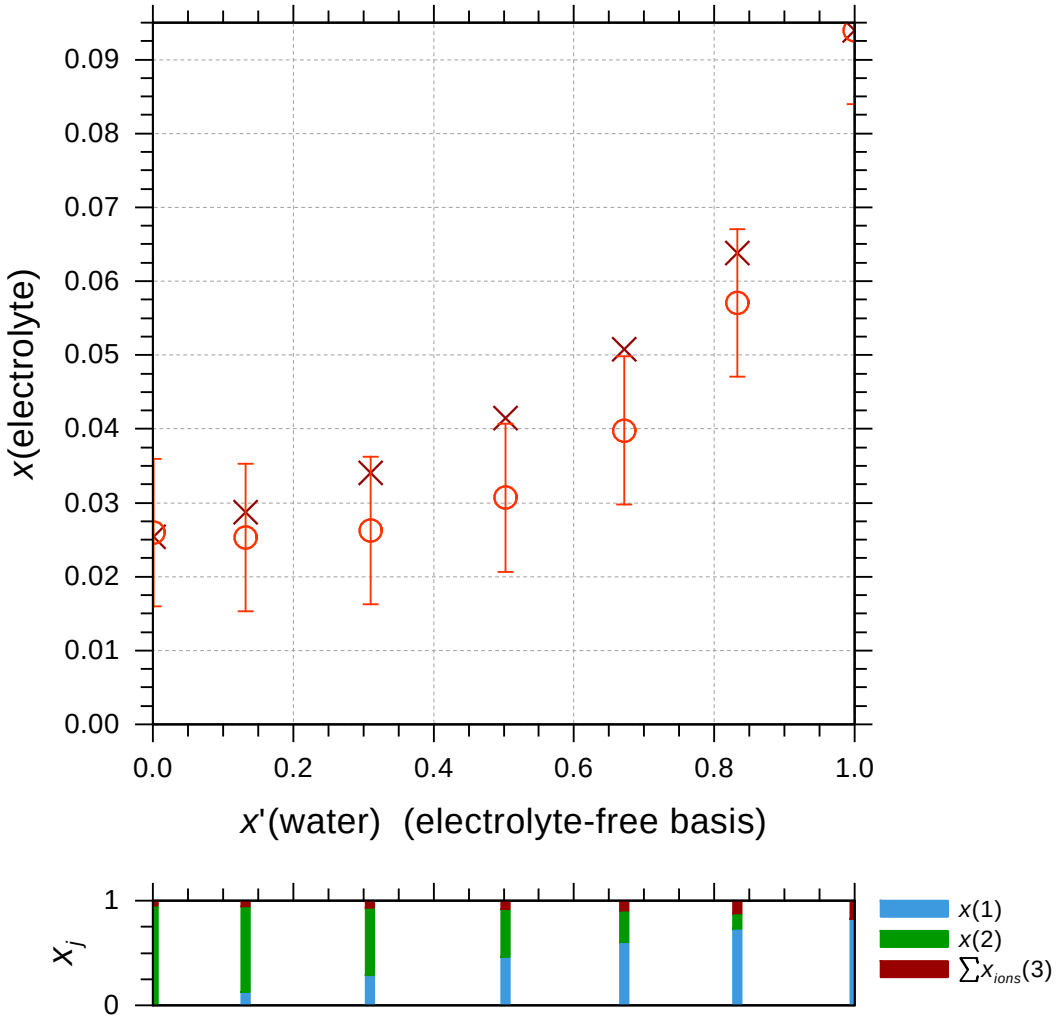
fval(0440) = 1.4280E+00

rel. contribution = 0.6790 %

Fig. S0347 (AIOMFAC_output_0398)

H_2O (1) + 2-Methoxyethanol (2) + KBr (3)

Temperature: 298 K

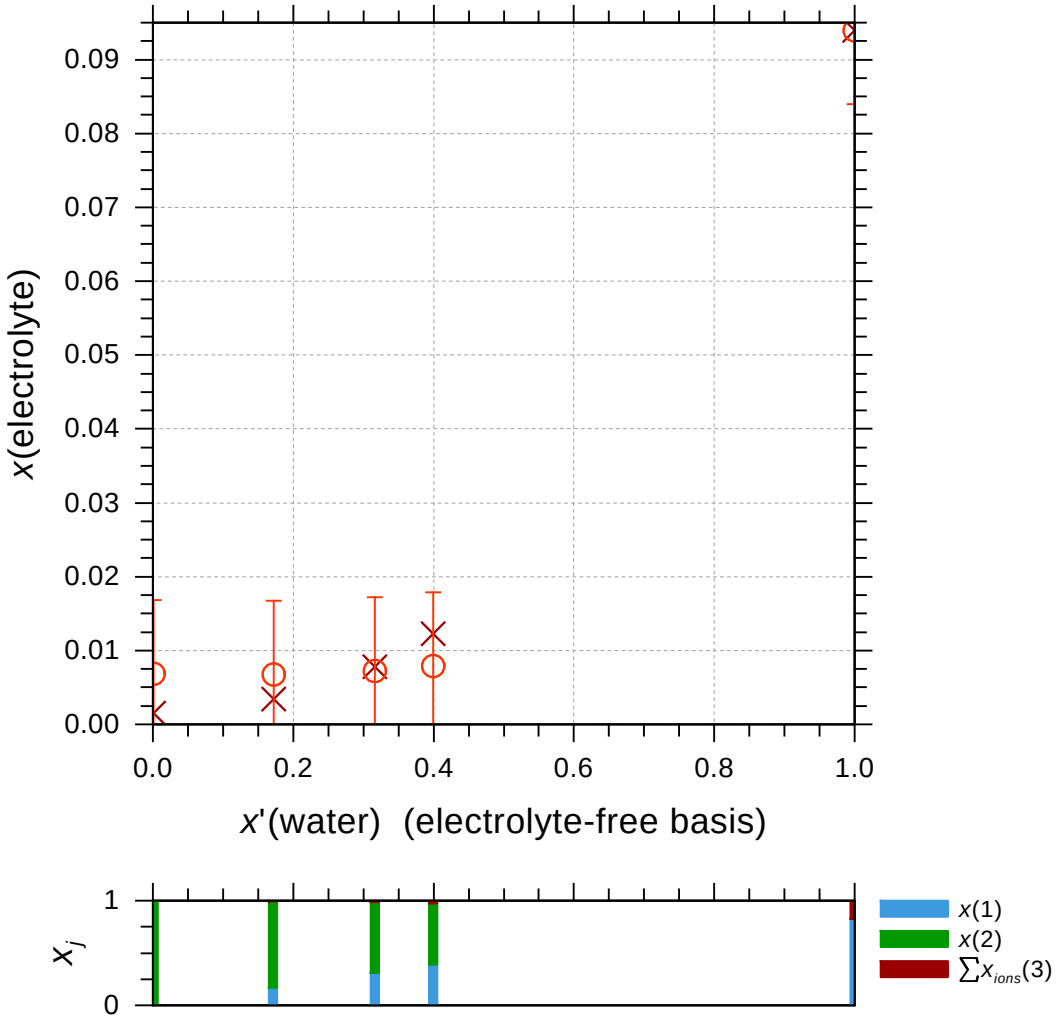


initial weighting of dataset:
w^{init}(0398) = 1.000
dataset contribution to F_{obj}:
fval(0398) = 1.2555E-01
rel. contribution = 0.0597 %

Fig. S0348 (AIOMFAC_output_0399)

H_2O (1) + 2-Butoxyethanol (2) + KBr (3)

Temperature: 298 K

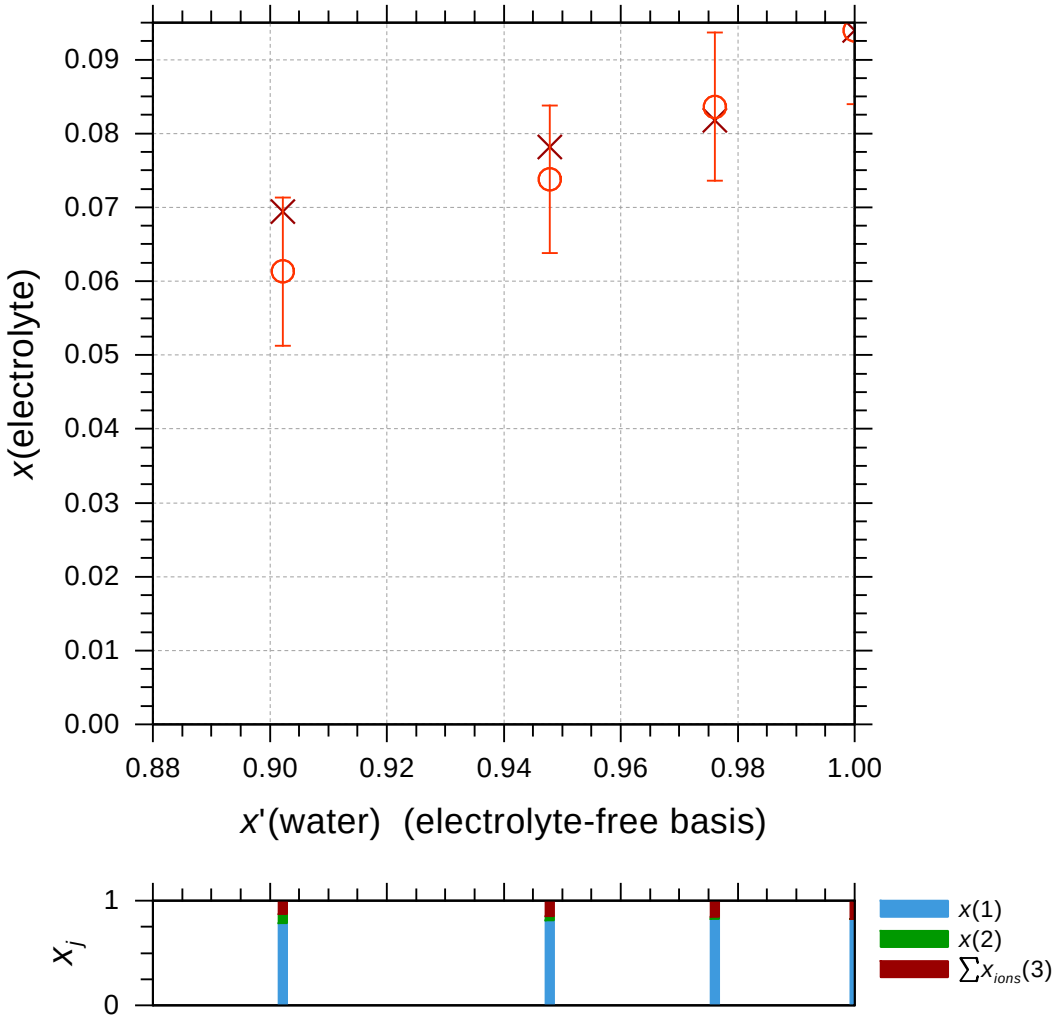


initial weighting of dataset:
$w^{init}(0399)$ = 1.000
dataset contribution to F_{obj}:
fval(0399) = 2.3637E-01
rel. contribution = 0.1019 %

Fig. S0349 (AIOMFAC_output_0967)

H_2O (1) + 1,4-Dioxane (2) + KBr (3)

Temperature: 298 K

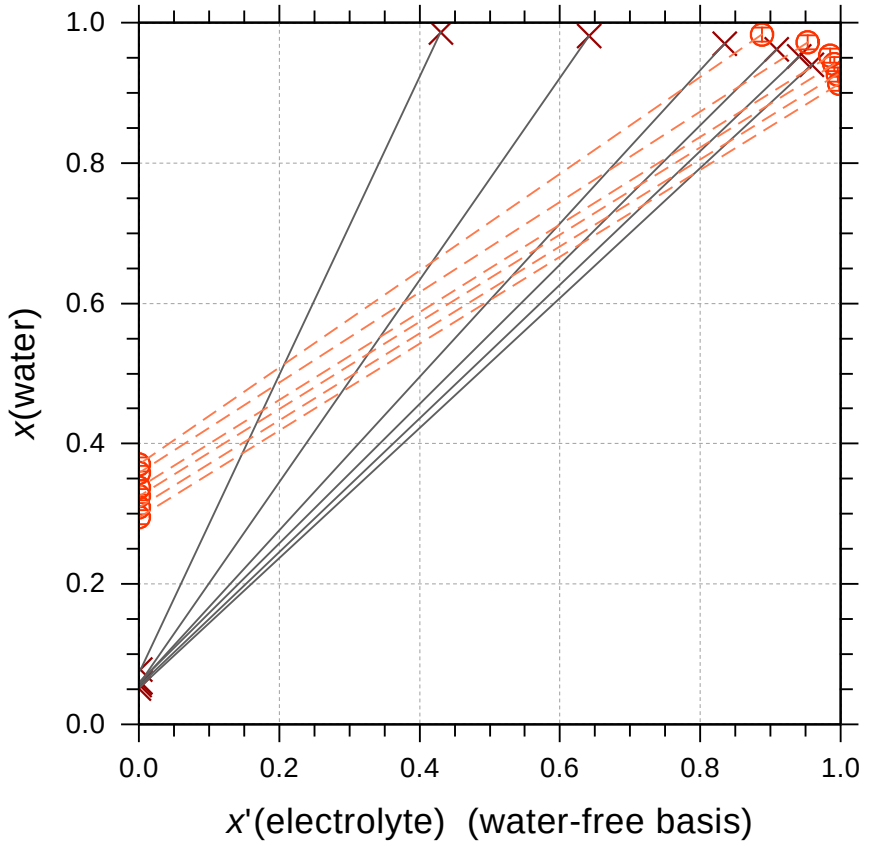


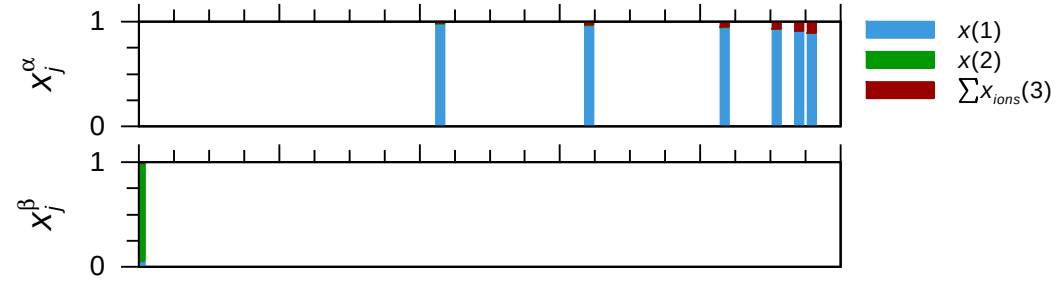
initial weighting of dataset:
$w^{init}(0967)$ = 1.000
dataset contribution to F_{obj}:
fval(0967) = 1.3467E-02
rel. contribution = 0.0064 %

Fig. S0350 (AIOMFAC_output_0365)

H_2O (1) + 2-Methoxy-2-methylpropane (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl+2-Methoxy-2-methylpropane+Water_LLE_Salabat

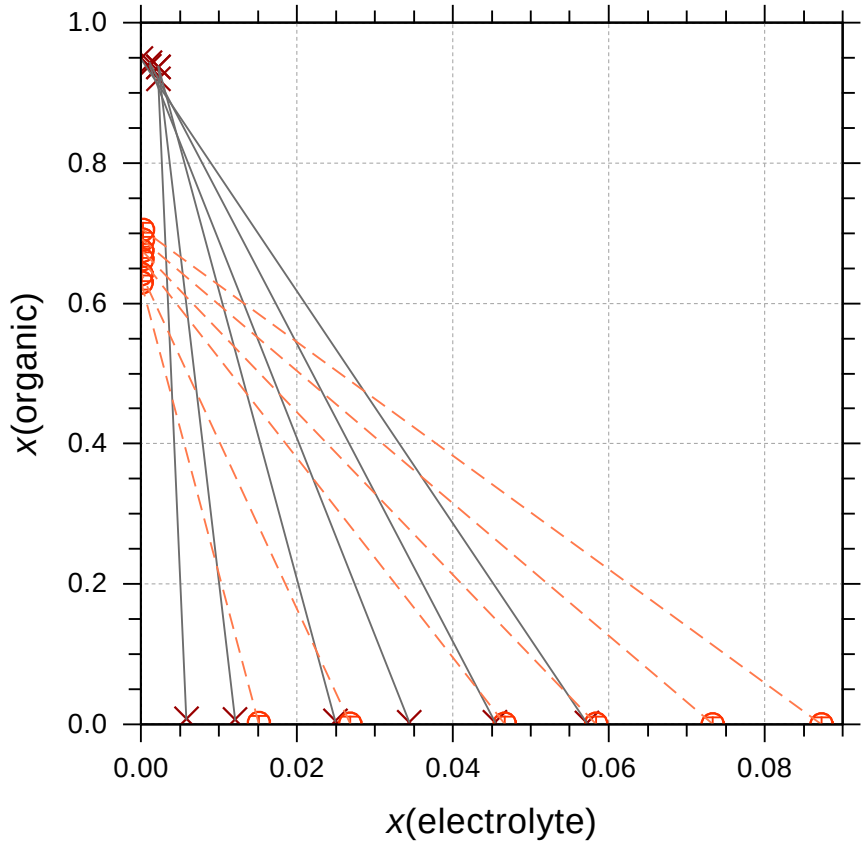
○ AIOMFAC calc. LLE composition

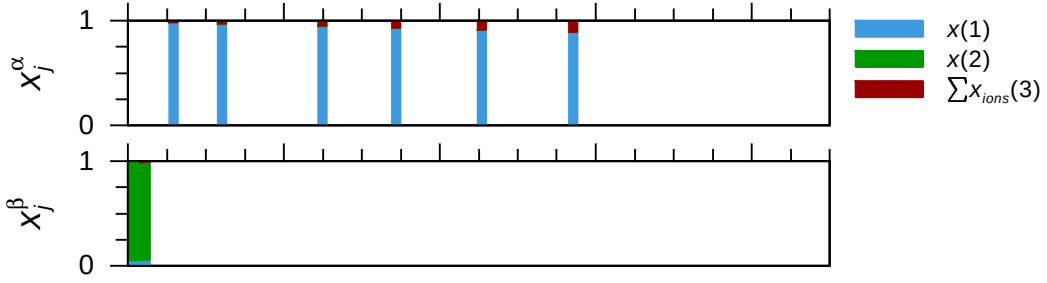
initial weighting of dataset:
w^{init}(0365) = 1.000
dataset contribution to F_{obj}:
fval(0365) = 2.9595E+00
rel. contribution = 1.4073 %

Fig. S0350a (AIOMFAC_output_0365)

H_2O (1) + 2-Methoxy-2-methylpropane (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl+2-Methoxy-2-methylpropane+Water_LLE_Salabat

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0365) = 1.000

dataset contribution to F_{obj}:

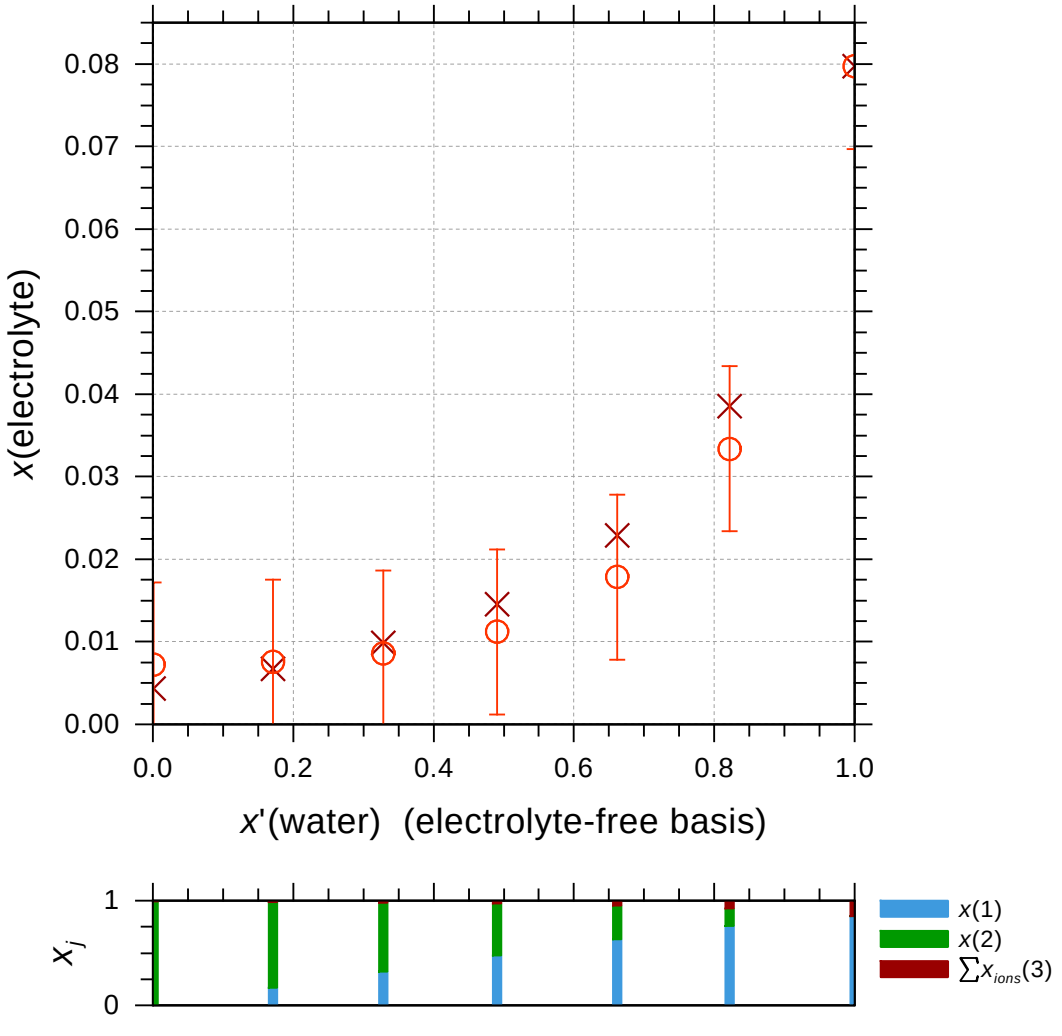
fval(0365) = 2.9595E+00

rel. contribution = 1.4073 %

Fig. S0351 (AIOMFAC_output_0394)

H_2O (1) + 2-Methoxyethanol (2) + KCl (3)

Temperature: 298 K

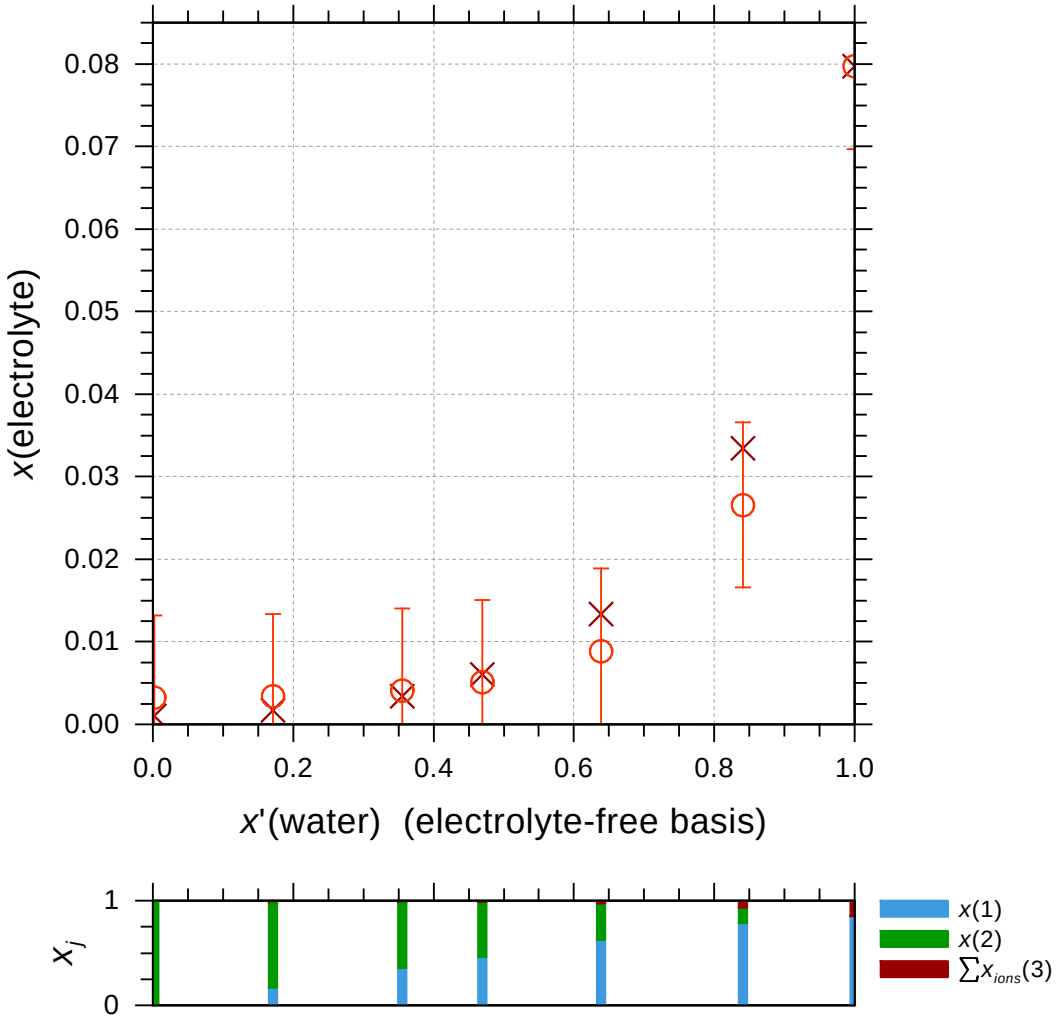


initial weighting of dataset:
$w^{init}(0394)$ = 1.000
dataset contribution to F_{obj}:
fval(0394) = 9.9260E-02
rel. contribution = 0.0472 %

Fig. S0352 (AIOMFAC_output_0395)

H_2O (1) + 2-Ethoxyethanol (2) + KCl (3)

Temperature: 298 K

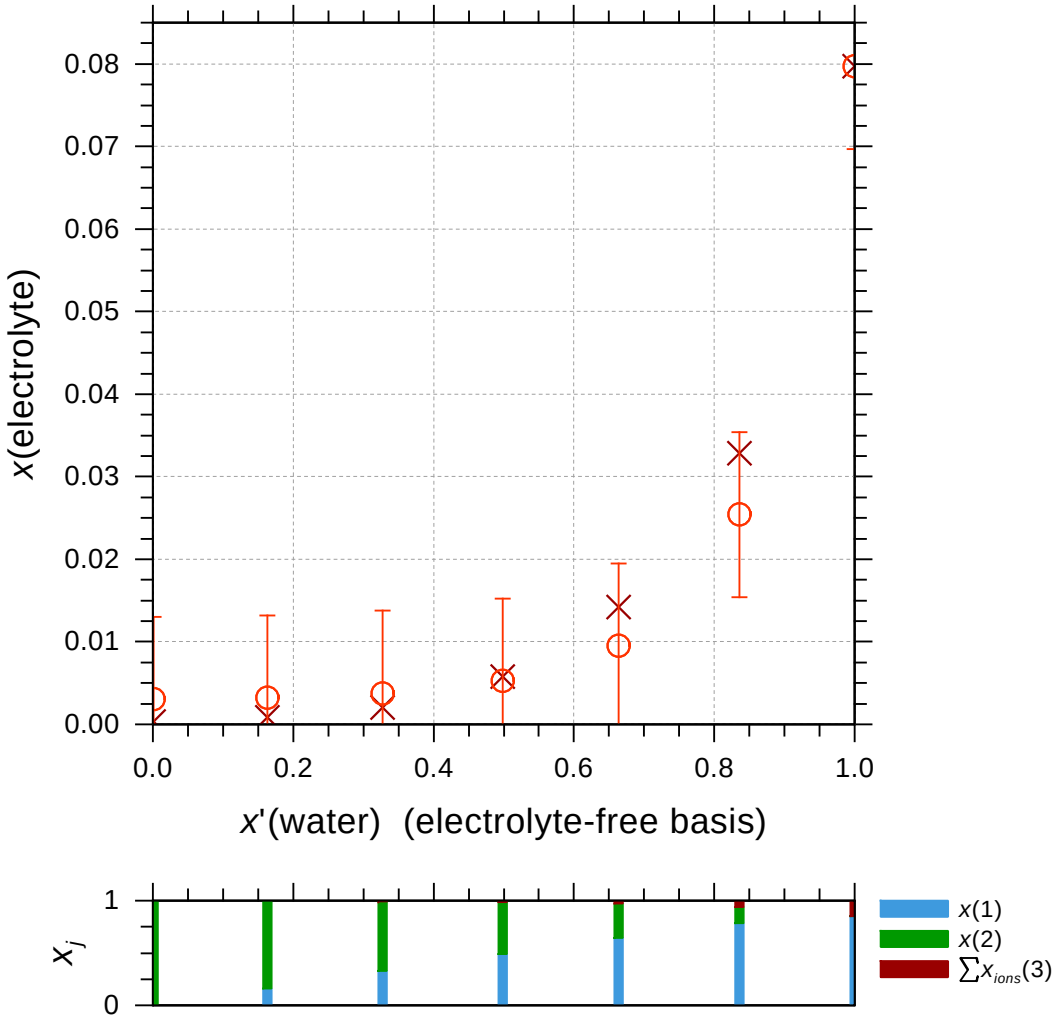


initial weighting of dataset:
$w^{init}(0395)$ = 1.000
dataset contribution to F_{obj}:
fval(0395) = 1.2909E-01
rel. contribution = 0.0614 %

Fig. S0353 (AIOMFAC_output_0396)

H_2O (1) + 1-Methoxy-2-propanol (2) + KCl (3)

Temperature: 298 K

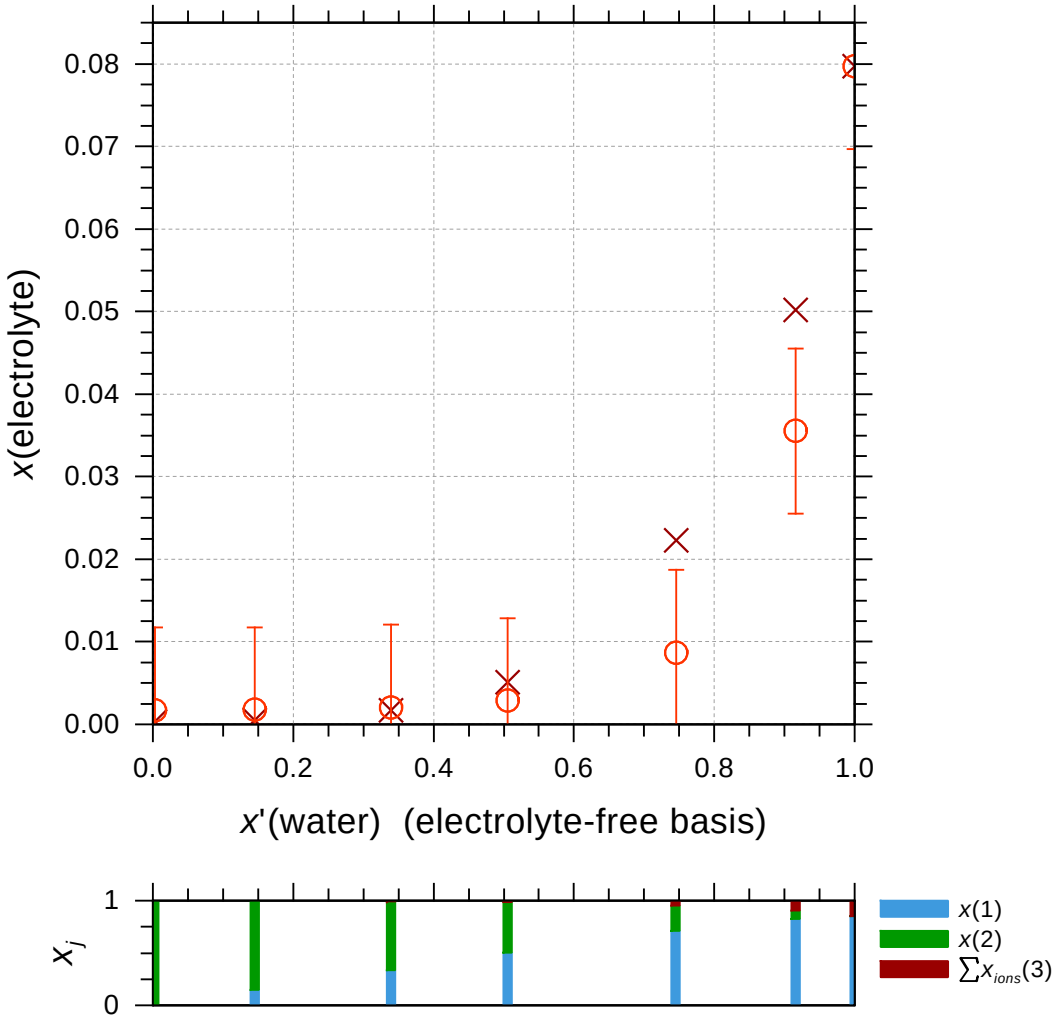


initial weighting of dataset:
$w^{init}(0396)$ = 1.000
dataset contribution to F_{obj}:
fval(0396) = 2.0352E-01
rel. contribution = 0.0968 %

Fig. S0354 (AIOMFAC_output_0397)

H_2O (1) + 2-Isopropoxyethanol (2) + KCl (3)

Temperature: 298 K

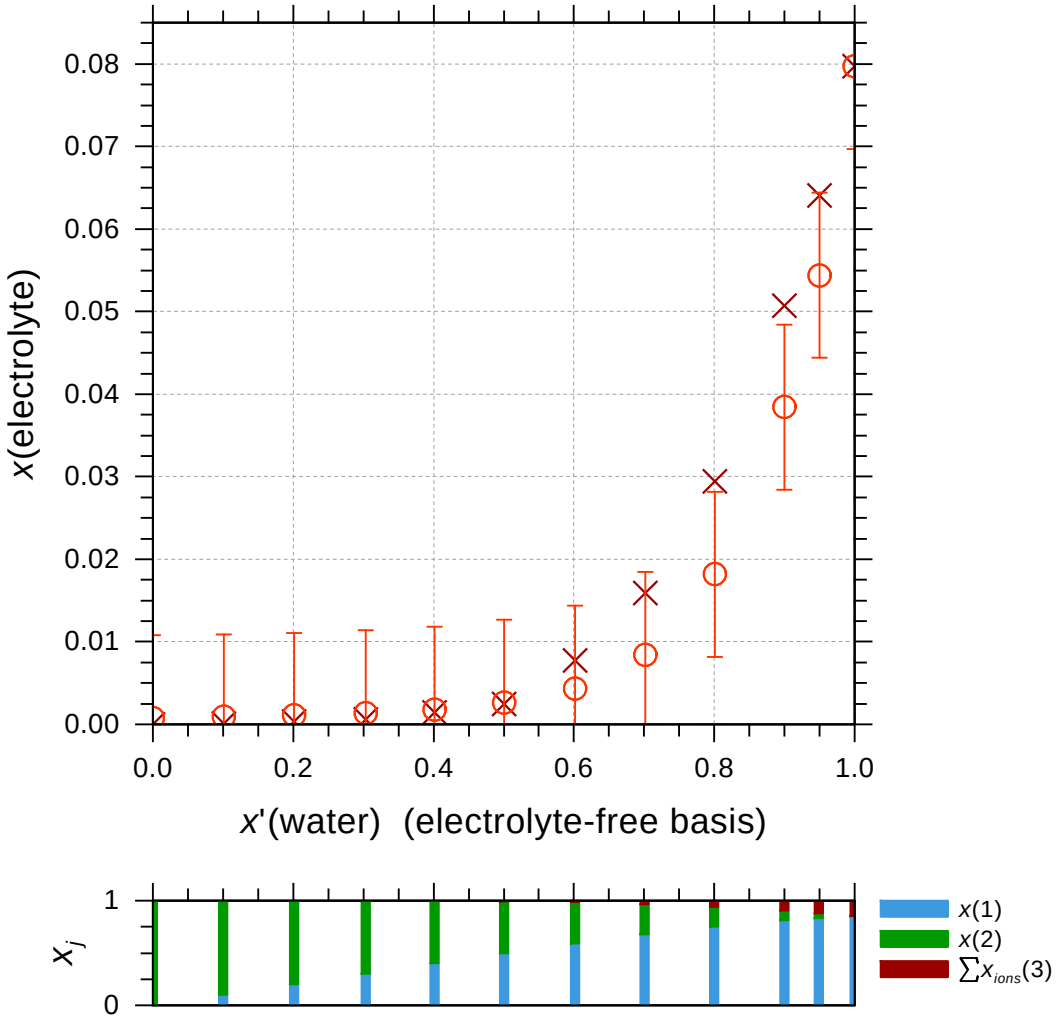


initial weighting of dataset:
$w^{init}(0397)$ = 1.000
dataset contribution to F_{obj}:
fval(0397) = 2.9281E-01
rel. contribution = 0.1392 %

Fig. S0355 (AIOMFAC_output_0444)

H_2O (1) + 1,4-Dioxane (2) + KCl (3)

Temperature: 298 K

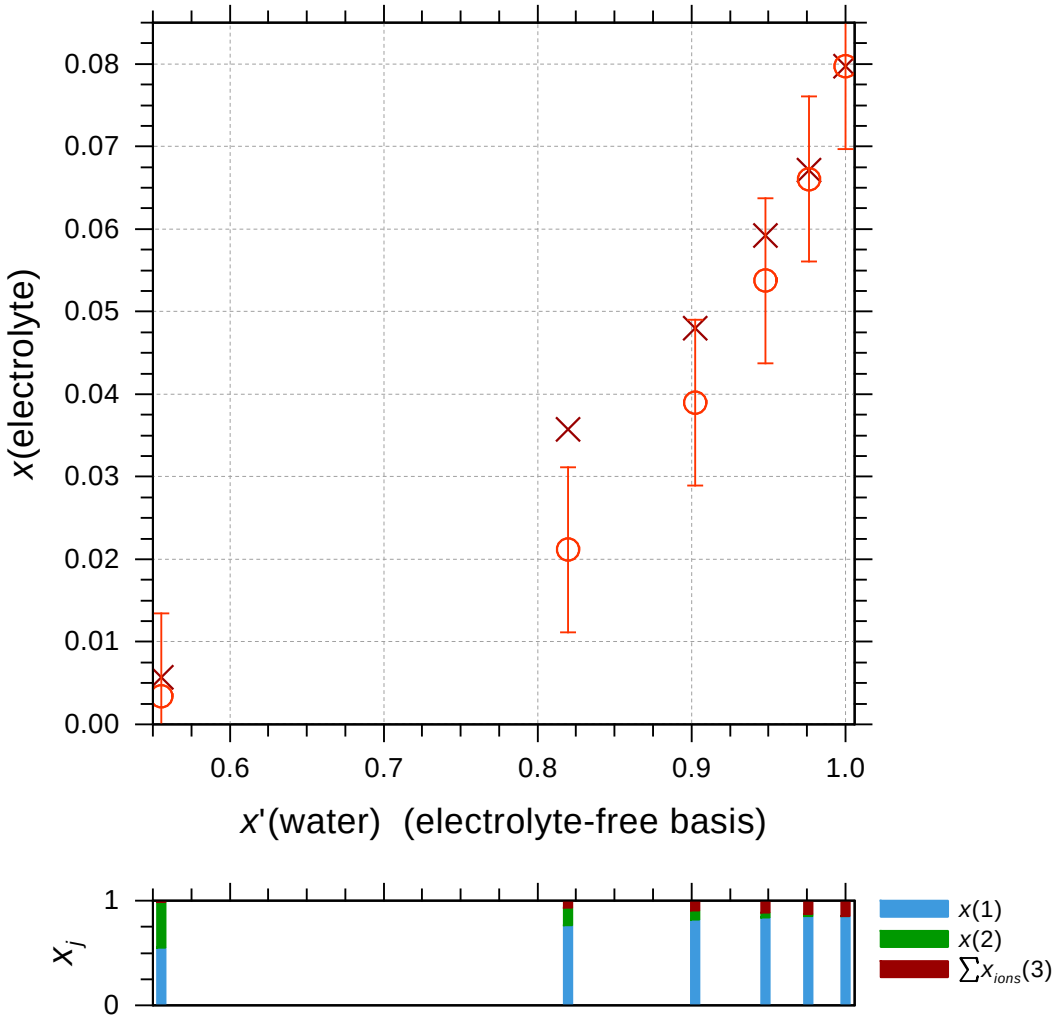


initial weighting of dataset:
$w^{init}(0444)$ = 1.000
dataset contribution to F_{obj}:
fval(0444) = 2.3675E-01
rel. contribution = 0.1126 %

Fig. S0356 (AIOMFAC_output_0966)

H_2O (1) + 1,4-Dioxane (2) + KCl (3)

Temperature: 298 K

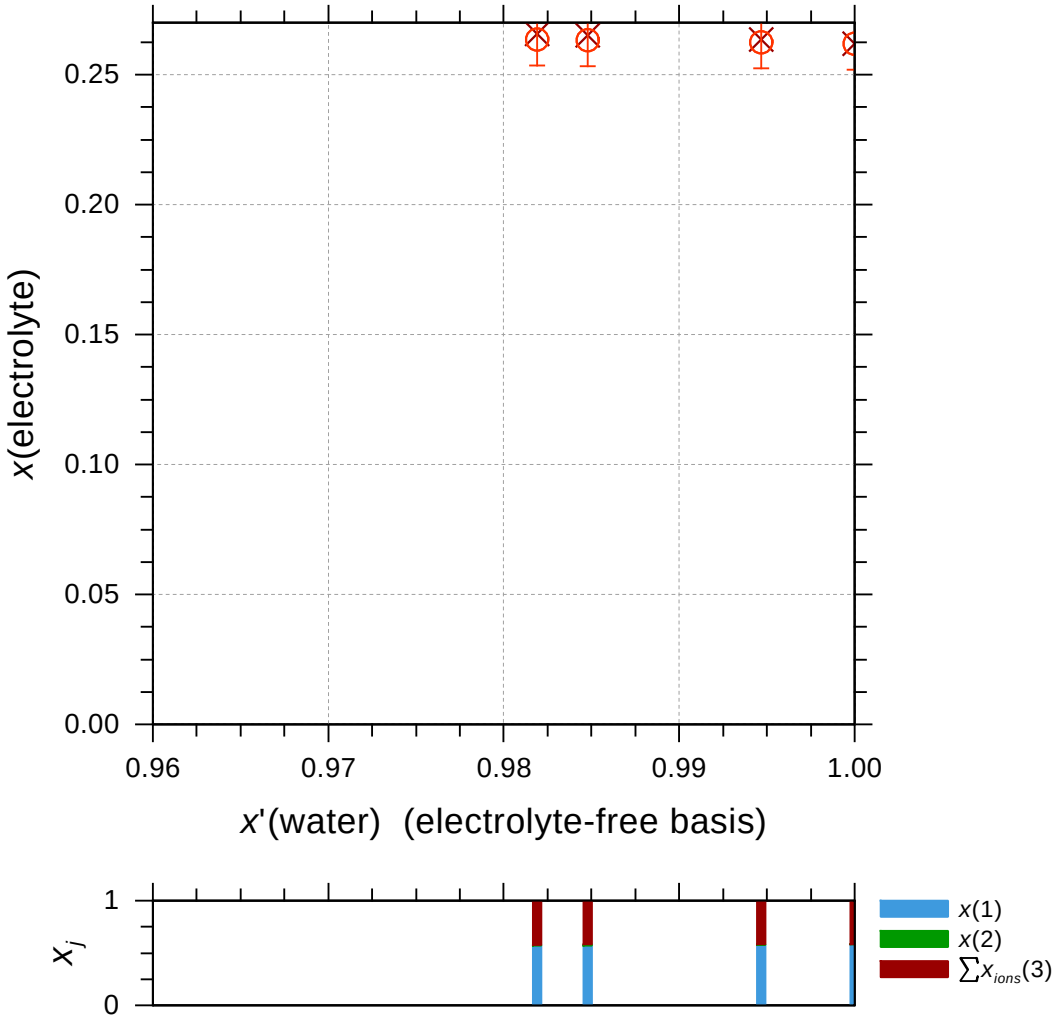


initial weighting of dataset:
w^{init}(0966) = 1.000
dataset contribution to F_{obj}:
fval(0966) = 1.5343E-01
rel. contribution = 0.0730 %

Fig. S0357 (AIOMFAC_output_0441)

H_2O (1) + 1,4-Dioxane (2) + LiCl (3)

Temperature: 298 K

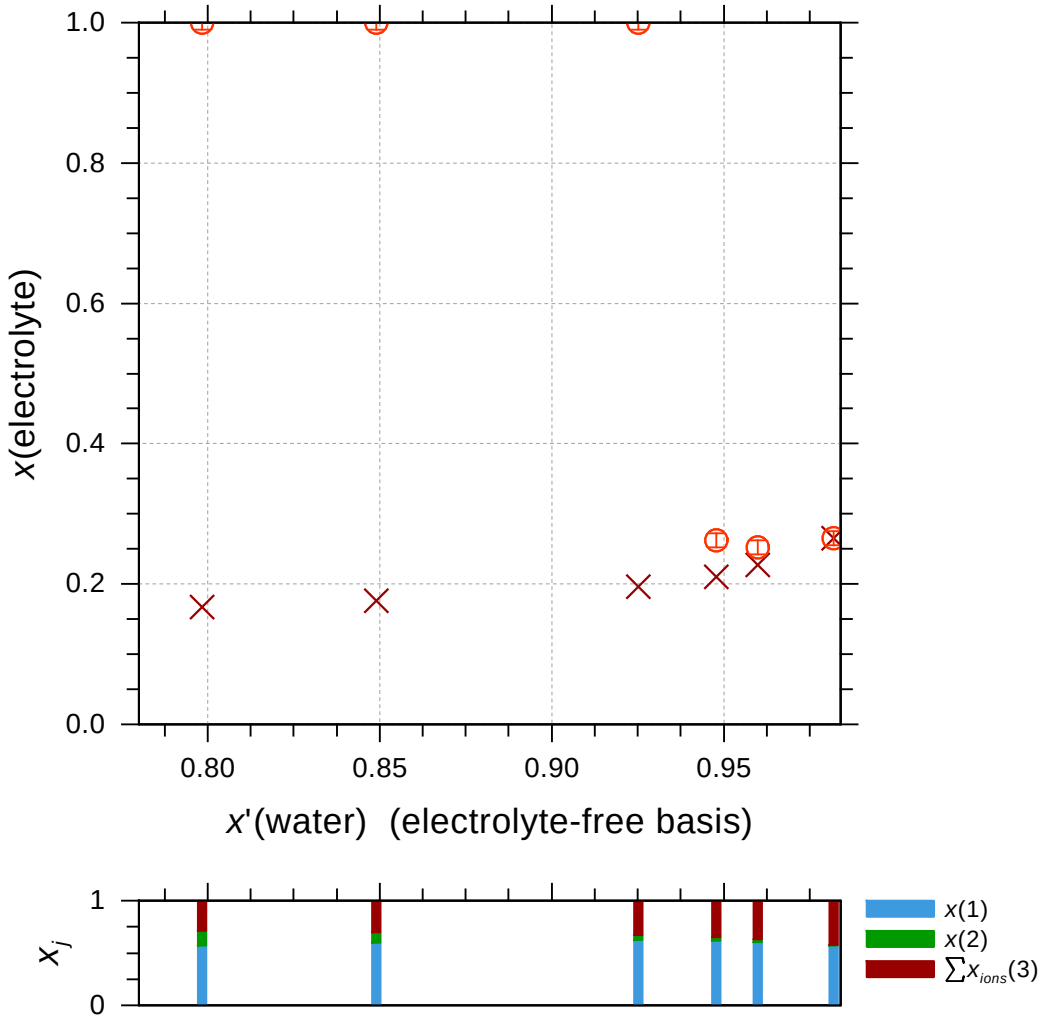


initial weighting of dataset:
$w^{init}(0441)$ = 0.020
dataset contribution to F_{obj}:
fval(0441) = 2.9051E-06
rel. contribution = 0.0000 %

Fig. S0358 (AIOMFAC_output_0442)

H_2O (1) + 1,4-Dioxane (2) + LiCl (3)

Temperature: 298 K

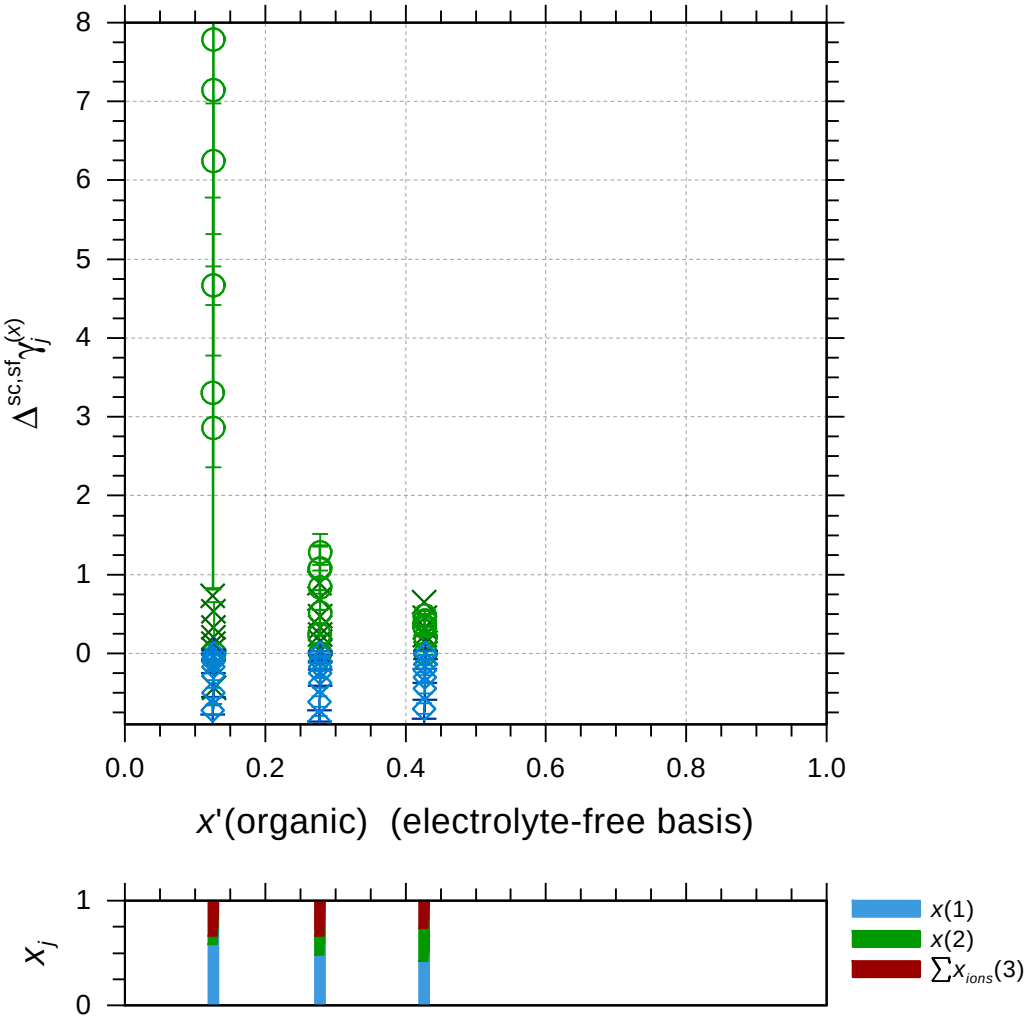


initial weighting of dataset:
$w^{init}(0442)$ = 0.020
dataset contribution to F_{obj}:
fval(0442) = 1.2476E+00
rel. contribution = 0.5933 %

Fig. S0359 (AIOMFAC_output_0930)

H_2O (1) + Tetrahydrofuran (2) + LiCl (3)

Temperature range: 337 -- 339 K



initial weighting of dataset:

$w^{init}(0930)$ = 0.200

dataset contribution to F_{obj}:

fval(0930) = 1.2845E+00

rel. contribution = 0.6108 %

Fig. S0360 (AIOMFAC_output_0364)

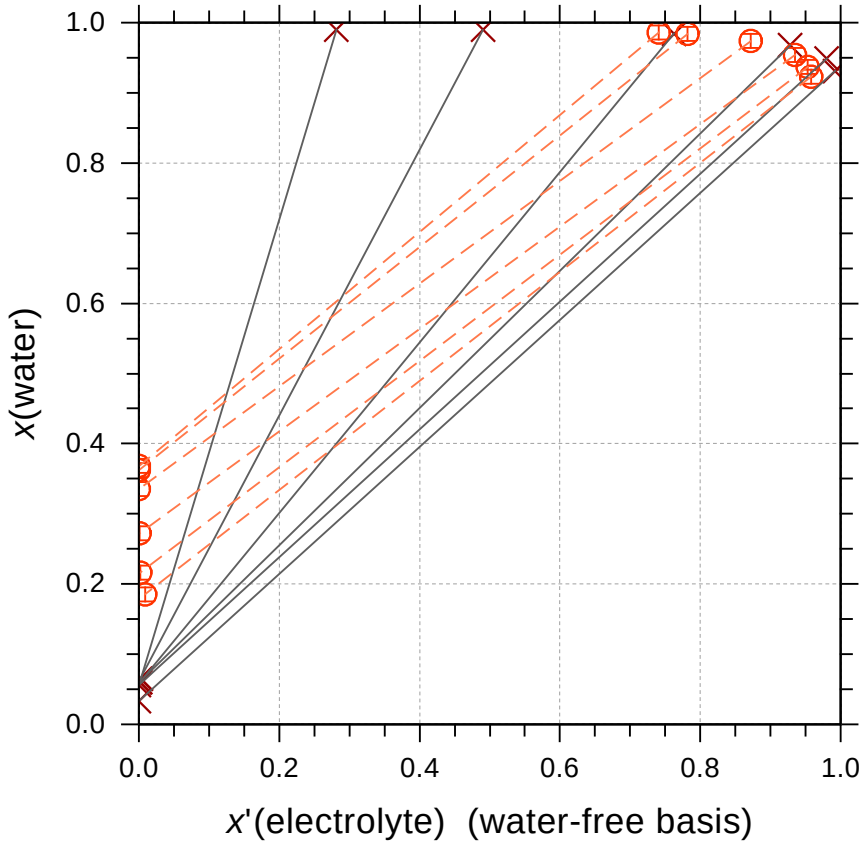
H_2O (1) + 2-Methoxy-2-methylpropane (2) + $MgCl_2$ (3)

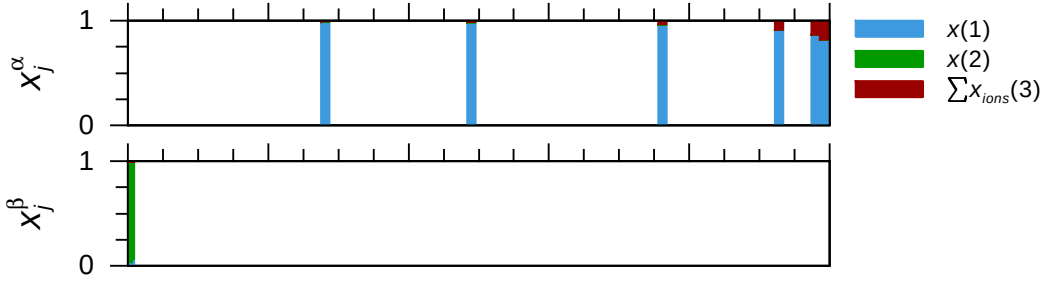
Temperature: 298 K

left y-axis:

× MgCl2+2-Methoxy-2-methylpropane+Water_LLE_Salabat

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

$w^{init}(0364)$ = 1.000

dataset contribution to F_{obj}:

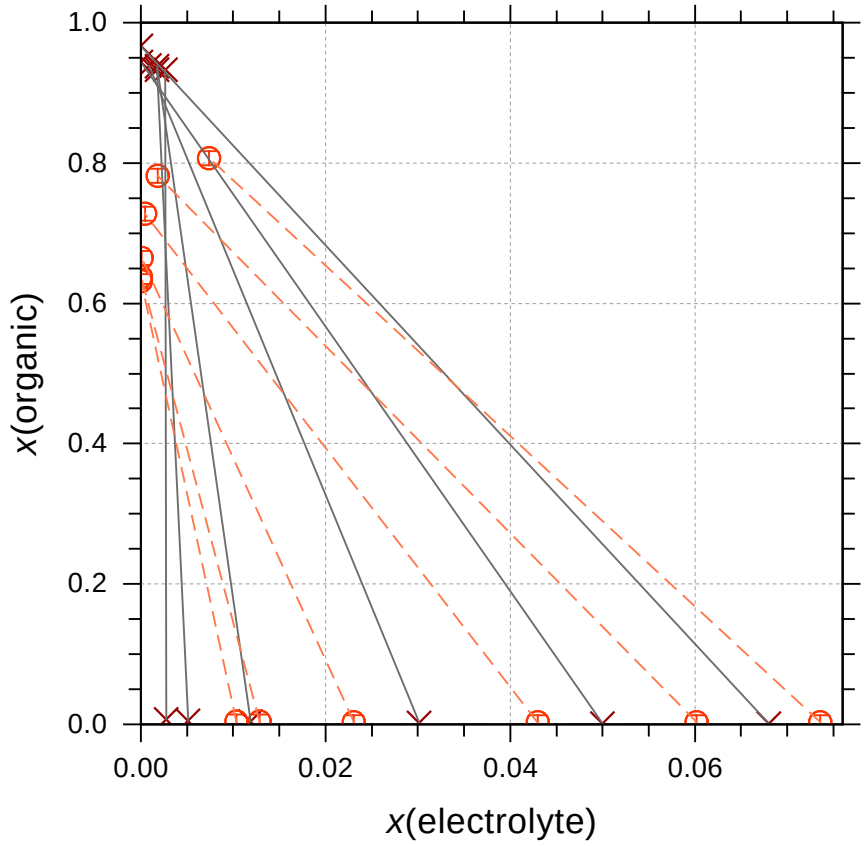
fval(0364) = 2.5087E+00

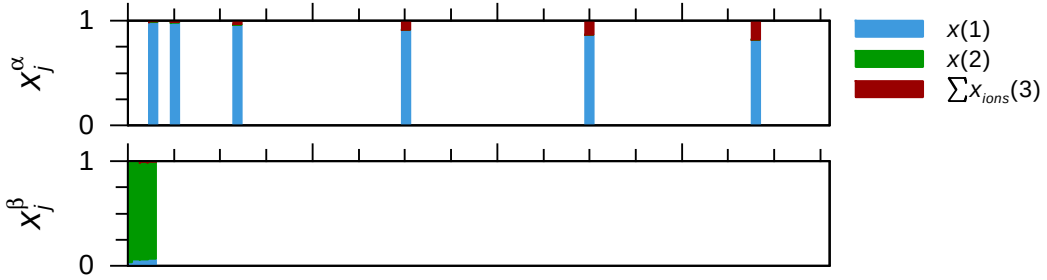
rel. contribution = 1.1930 %

Fig. S0360a (AIOMFAC_output_0364)

H_2O (1) + 2-Methoxy-2-methylpropane (2) + $MgCl_2$ (3)

Temperature: 298 K





left y-axis:

× MgCl2+2-Methoxy-2-methylpropane+Water_LLE_Salabat

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0364) = 1.000

dataset contribution to F_{obj}:

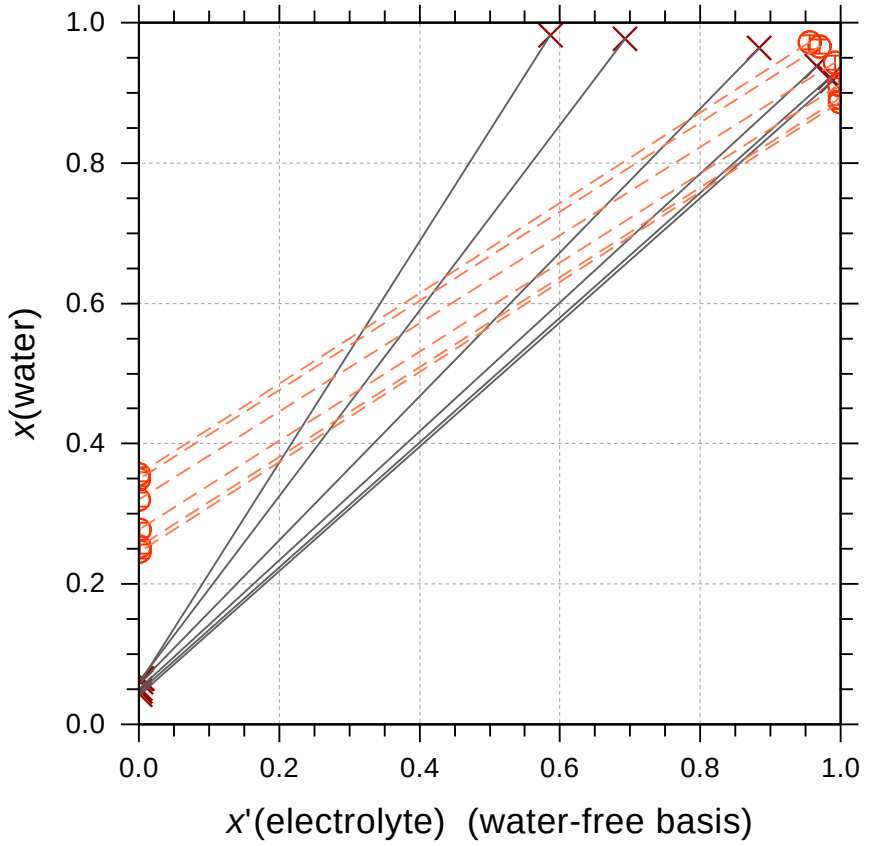
fval(0364) = 2.5087E+00

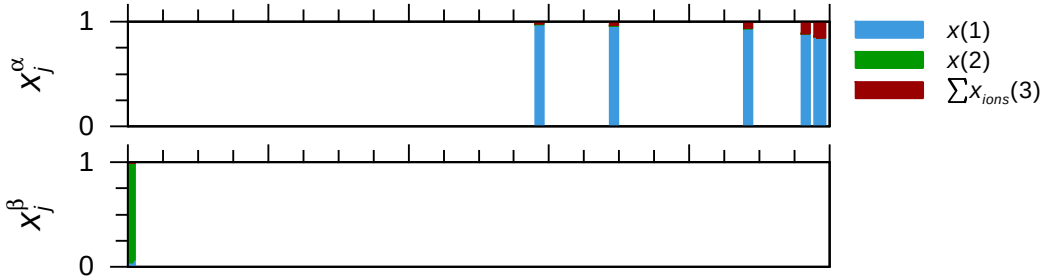
rel. contribution = 1.1930 %

Fig. S0361 (AIOMFAC_output_0366)

H_2O (1) + 2-Methoxy-2-methylpropane (2) + NaCl (3)

Temperature: 298 K





left y-axis:

× NaCl+2-Methoxy-2-methylpropane+Water_LLE_Salabat

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0366) = 1.000

dataset contribution to F_{obj}:

fval(0366) = 3.0639E+00

rel. contribution = 1.4570 %

Fig. S0361a (AIOMFAC_output_0366)

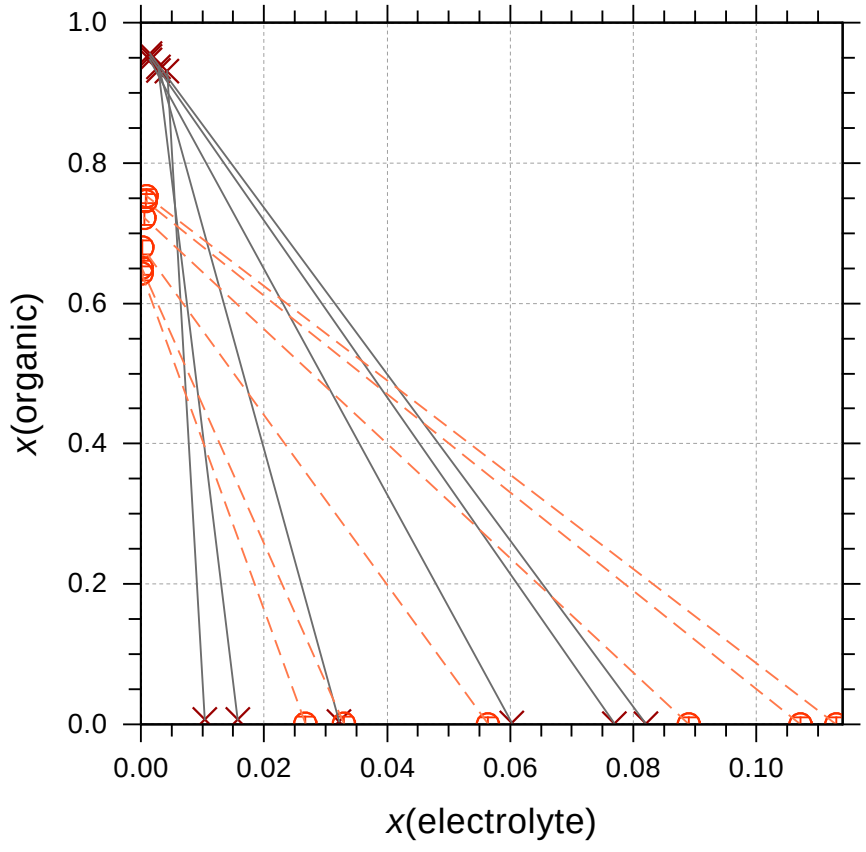
H_2O (1) + 2-Methoxy-2-methylpropane (2) + NaCl (3)

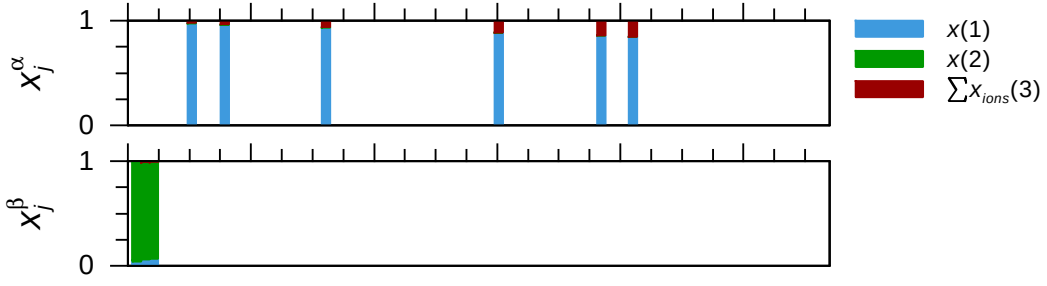
Temperature: 298 K

left y-axis:

× NaCl+2-Methoxy-2-methylpropane+Water_LLE_Salabat

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0366) = 1.000

dataset contribution to F_{obj}:

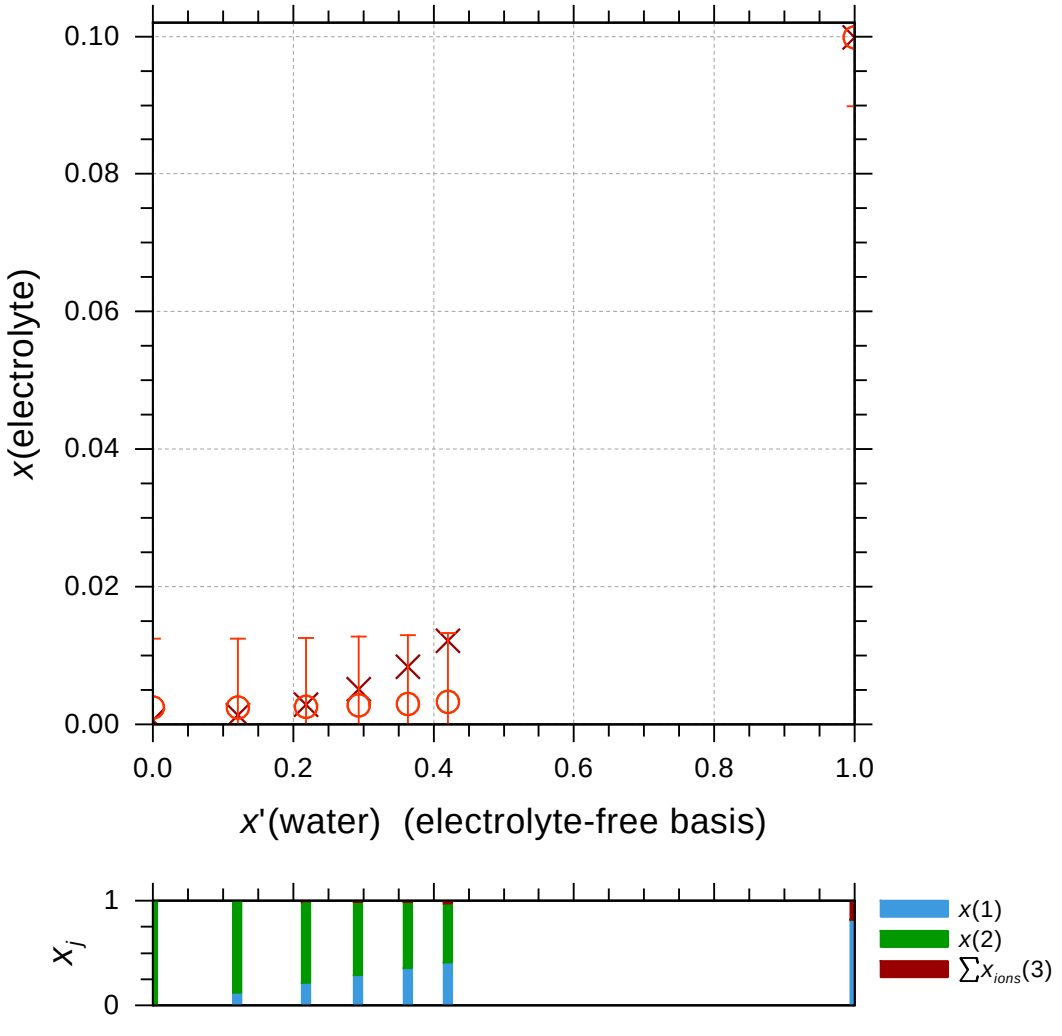
fval(0366) = 3.0639E+00

rel. contribution = 1.4570 %

Fig. S0362 (AIOMFAC_output_0401)

H_2O (1) + 2-Butoxyethanol (2) + NaCl (3)

Temperature: 298 K

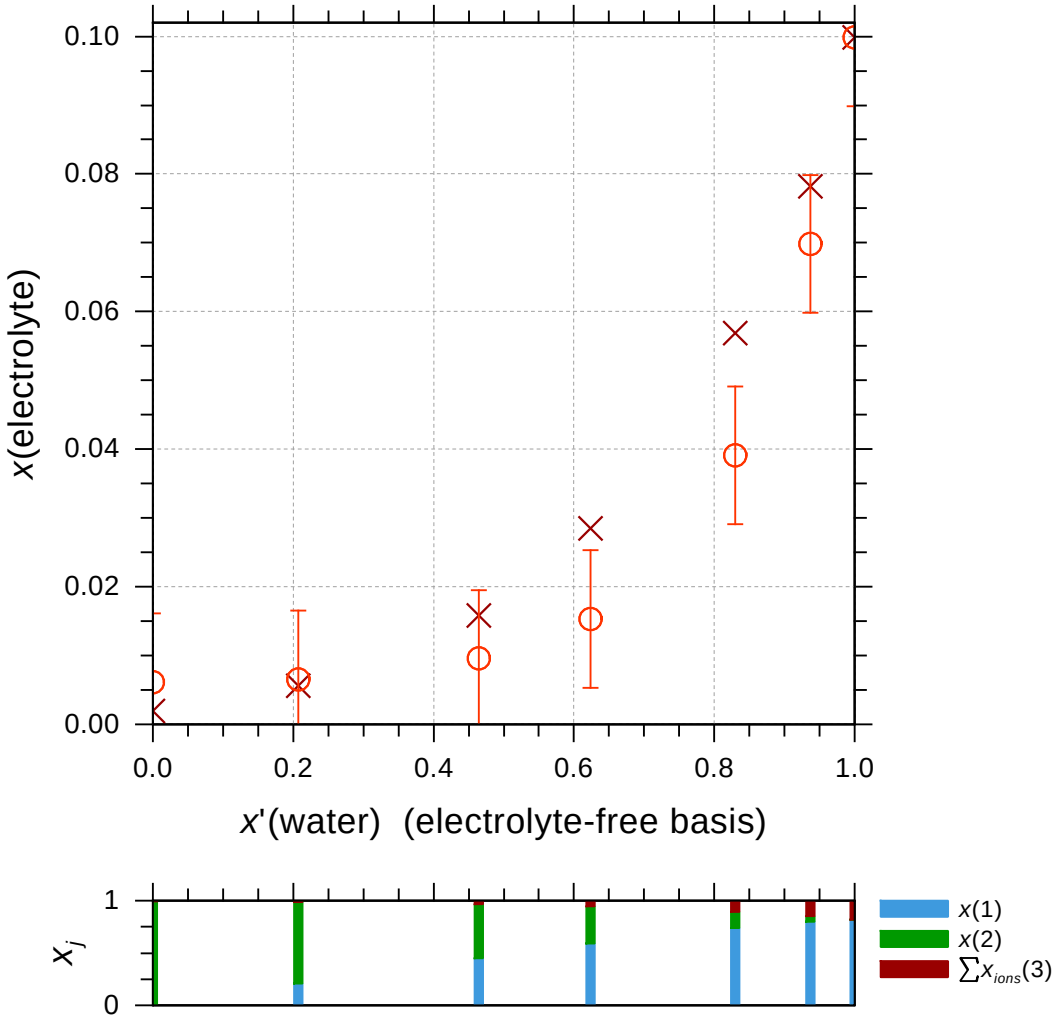


initial weighting of dataset:
$w^{init}(0401)$ = 1.000
dataset contribution to F_{obj}:
fval(0401) = 3.0990E-01
rel. contribution = 0.1474 %

Fig. S0363 (AIOMFAC_output_0402)

H_2O (1) + 2-Ethoxyethanol (2) + NaCl (3)

Temperature: 298 K

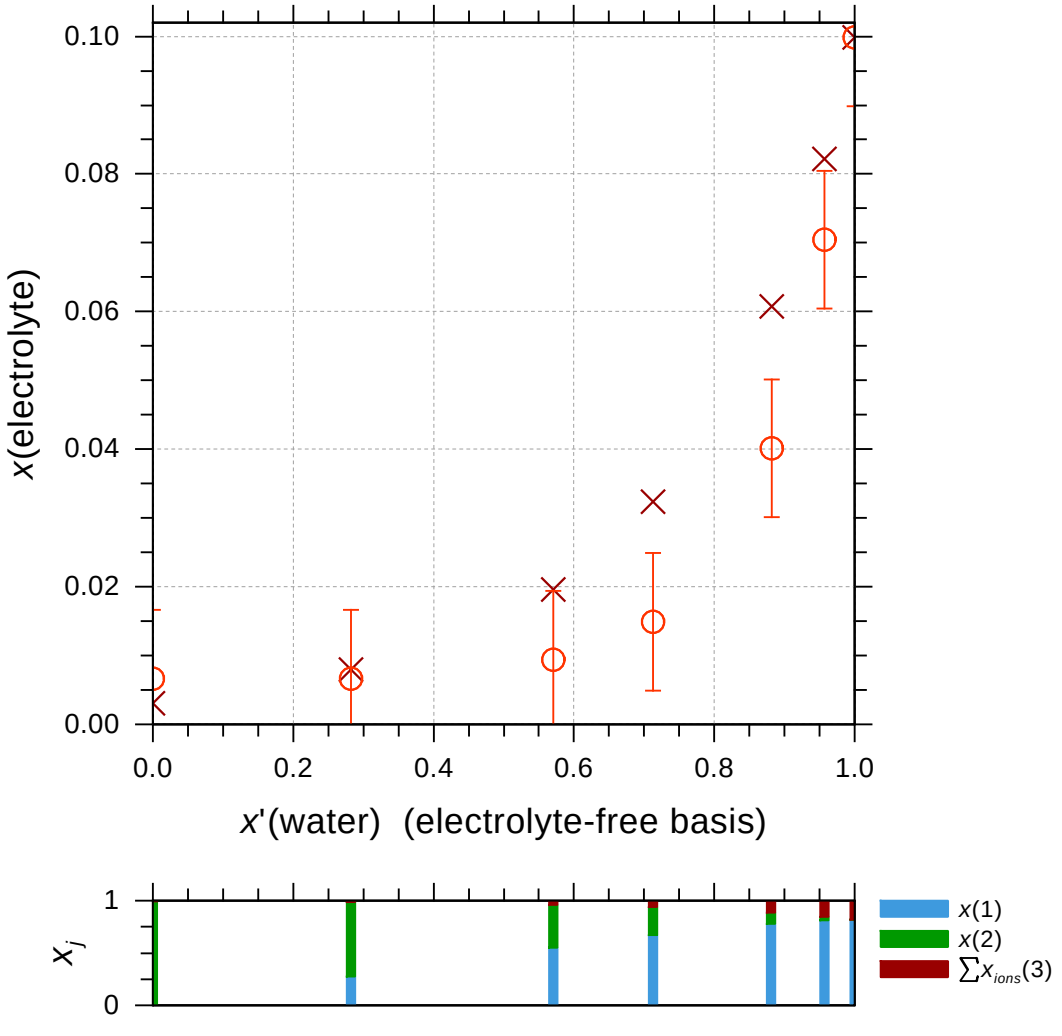


initial weighting of dataset:
w^{init}(0402) = 1.000
dataset contribution to F_{obj}:
fval(0402) = 3.8421E-01
rel. contribution = 0.1827 %

Fig. S0364 (AIOMFAC_output_0403)

H_2O (1) + 2-(2-ethoxyethoxy)ethanol (2) + NaCl (3)

Temperature: 298 K

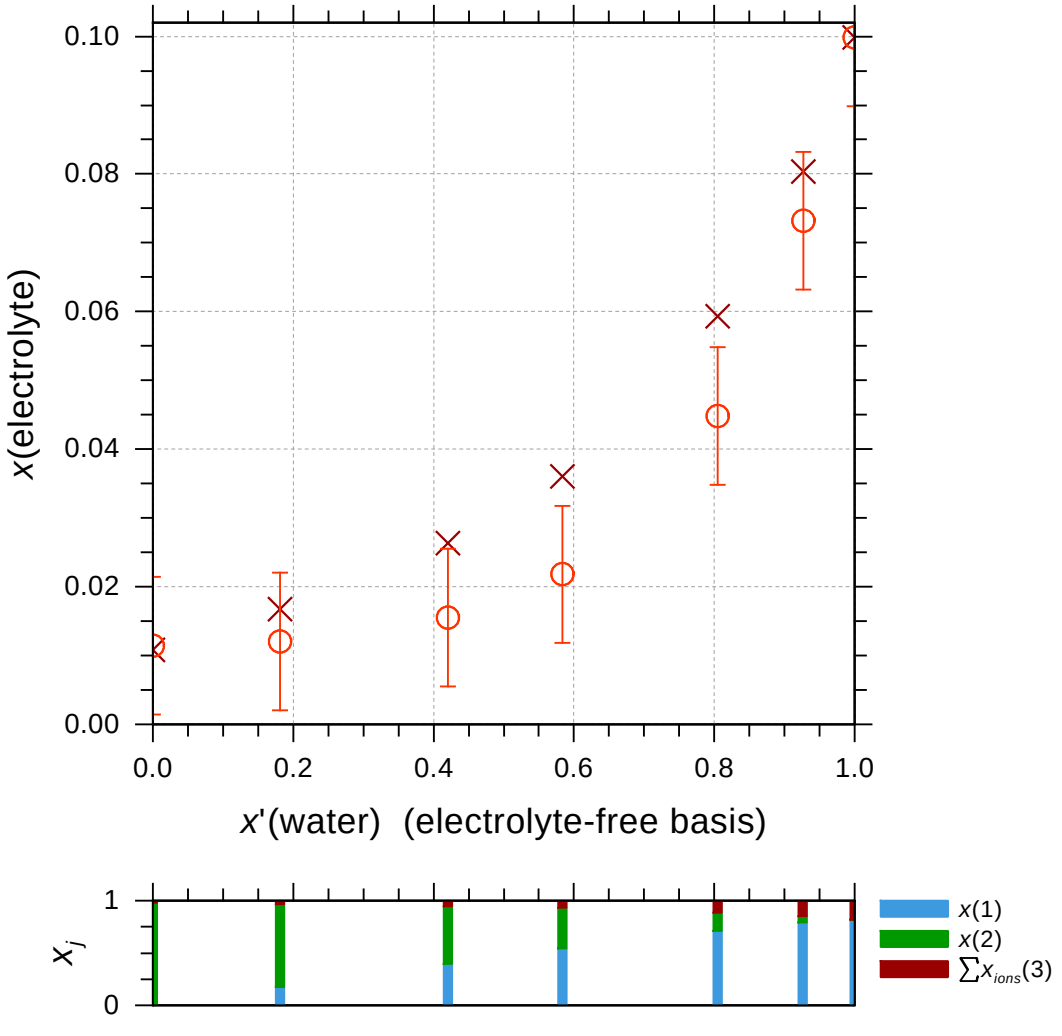


initial weighting of dataset:
w^{init}(0403) = 1.000
dataset contribution to F_{obj}:
fval(0403) = 4.7349E-01
rel. contribution = 0.2252 %

Fig. S0365 (AIOMFAC_output_0404)

H_2O (1) + 2-Methoxyethanol (2) + NaCl (3)

Temperature: 298 K

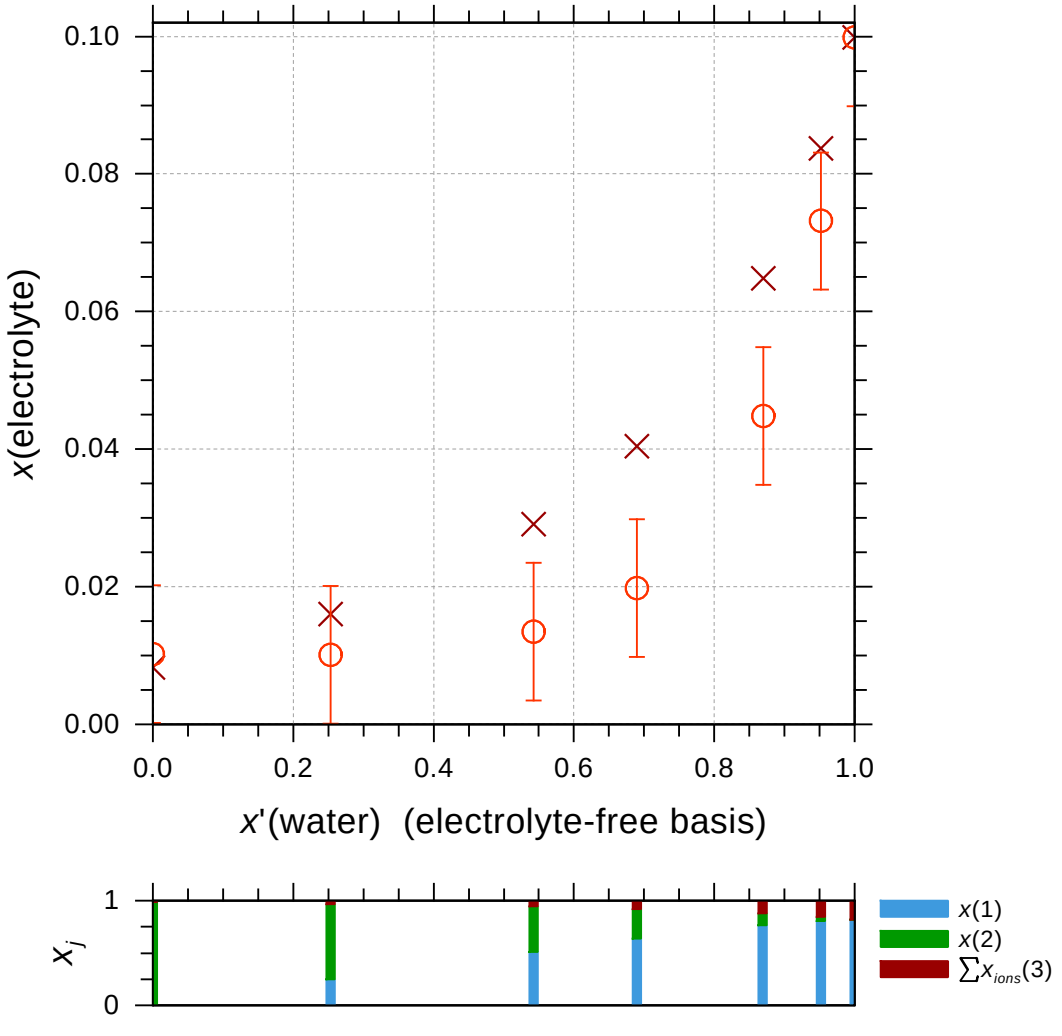


initial weighting of dataset:
$w^{init}(0404)$ = 1.000
dataset contribution to F_{obj}:
fval(0404) = 2.6844E-01
rel. contribution = 0.1277 %

Fig. S0366 (AIOMFAC_output_0405)

H_2O (1) + 2-(2-methoxyethoxy)ethanol (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:
$w^{init}(0405)$ = 1.000
dataset contribution to F_{obj}:
fval(0405) = 4.7689E-01
rel. contribution = 0.2268 %

Fig. S0367 (AIOMFAC_output_0406)

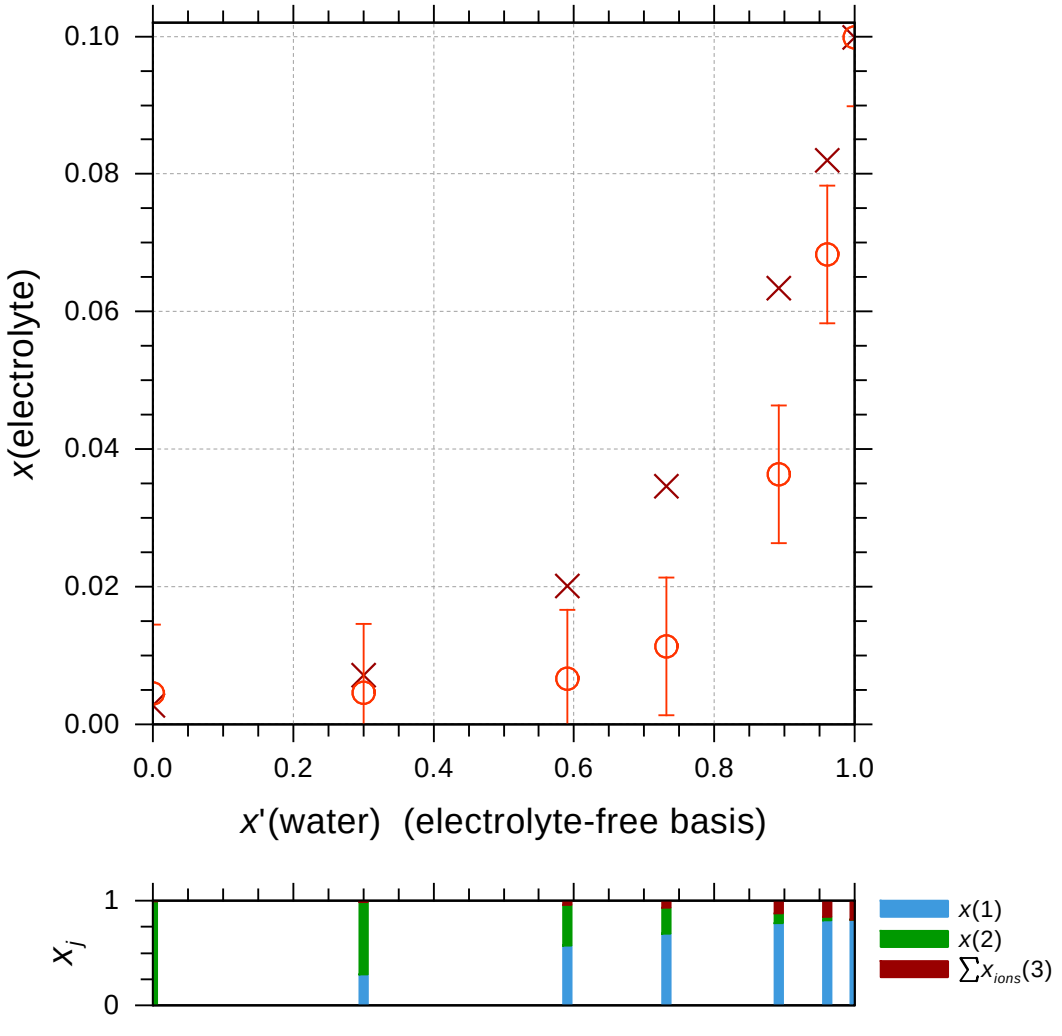
H_2O (1) + 1-(2-methoxypropoxy)-2-propanol (2) + NaCl (3)

Temperature: 298 K

left y-axis:

× NaCl+1-(2-methoxypropoxy)-2-propanol+Water_SLE_Raridon

○ AIOMFAC calc. SLE composition

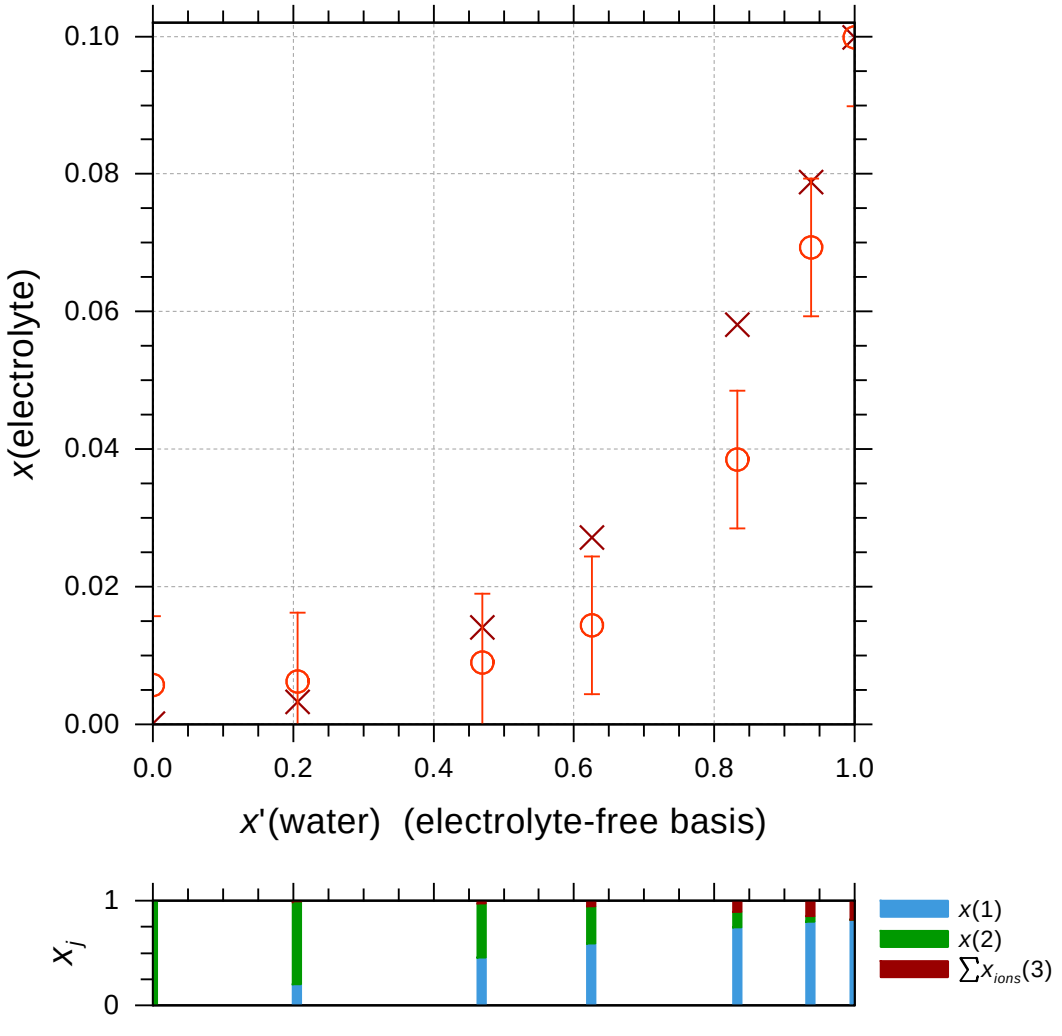


initial weighting of dataset:
w^{init}(0406) = 1.000
dataset contribution to F_{obj}:
fval(0406) = 6.7543E-01
rel. contribution = 0.3212 %

Fig. S0368 (AIOMFAC_output_0407)

H_2O (1) + 2-Methoxypropanol (2) + NaCl (3)

Temperature: 298 K

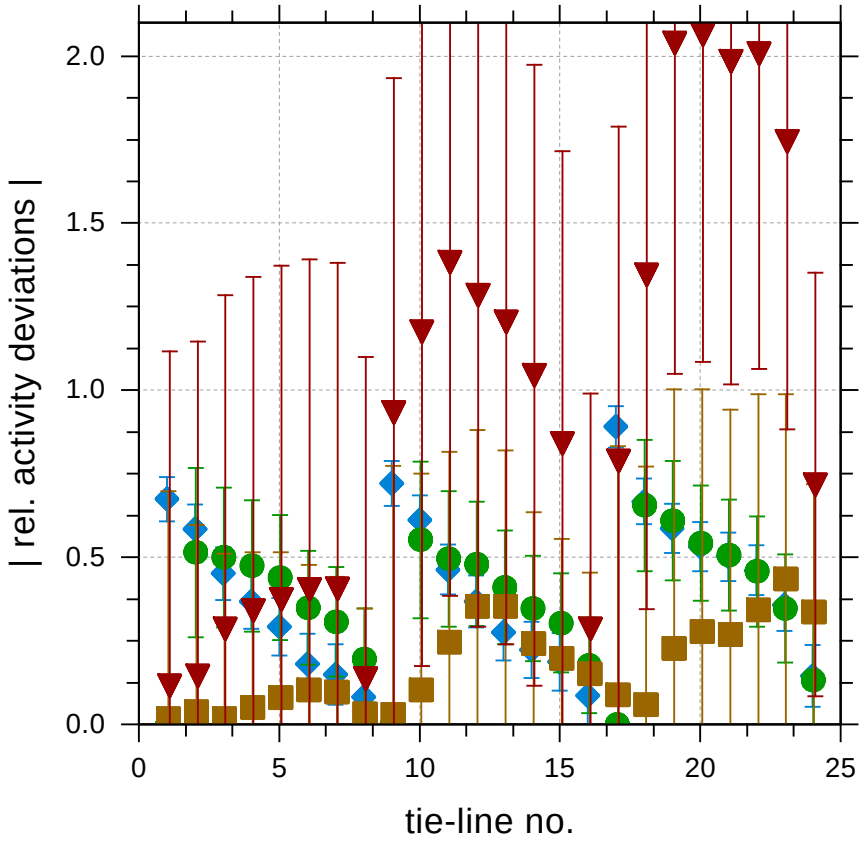


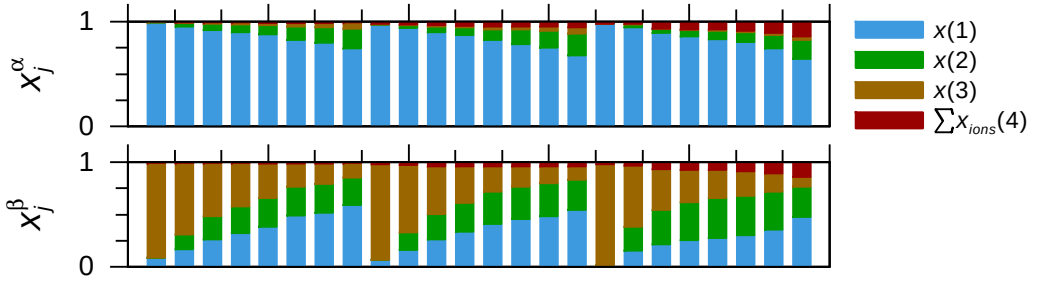
initial weighting of dataset:
$w^{init}(0407)$ = 1.000
dataset contribution to F_{obj}:
fval(0407) = 6.2709E-01
rel. contribution = 0.2982 %

Fig. S0369 (AIOMFAC_output_0427)

H_2O (1) + Acetic_acid (2) + 2-Methoxy-2-methylpropane (3) + NaCl (4)

Temperature: 298 K





left y-axis:

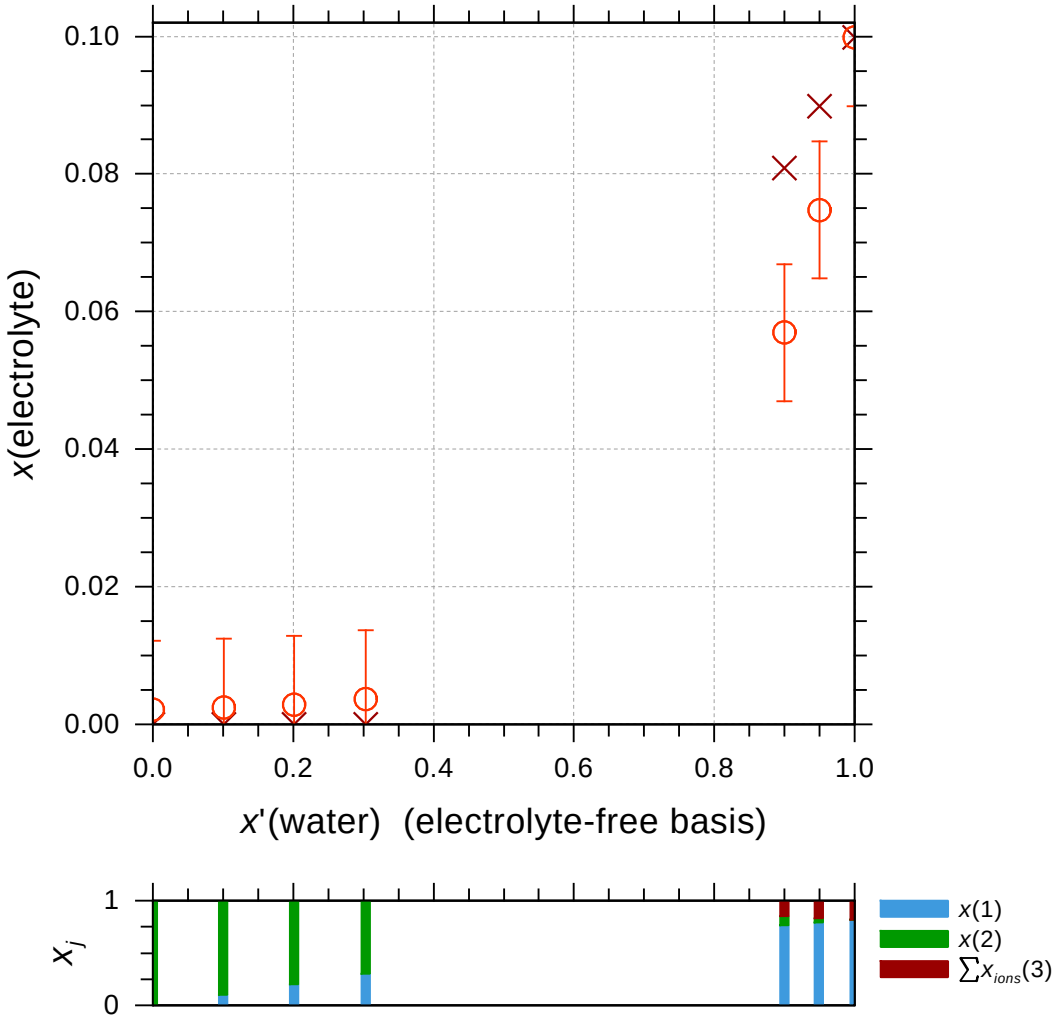
- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

initial weighting of dataset:
w^{init}(0427) = 0.100
dataset contribution to F_{obj}:
fval(0427) = 8.8737E-01
rel. contribution = 0.4220 %

Fig. S0370 (AIOMFAC_output_0443)

H_2O (1) + 1,4-Dioxane (2) + NaCl (3)

Temperature: 298 K

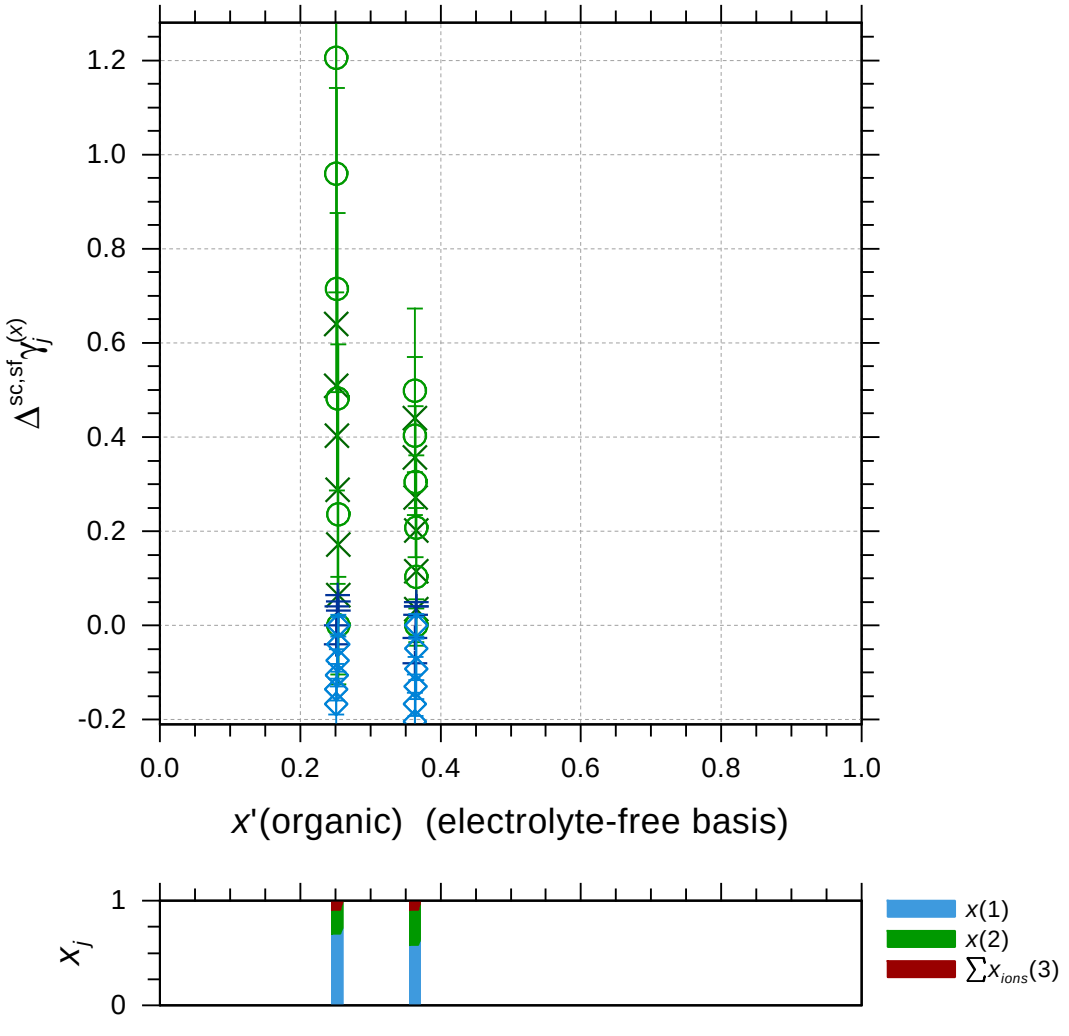


initial weighting of dataset:
w^{init}(0443) = 1.000
dataset contribution to F_{obj}:
fval(0443) = 4.1161E-01
rel. contribution = 0.1957 %

Fig. S0371 (AIOMFAC_output_0929)

H_2O (1) + Tetrahydrofuran (2) + NaCl (3)

Temperature range: 337 -- 337 K

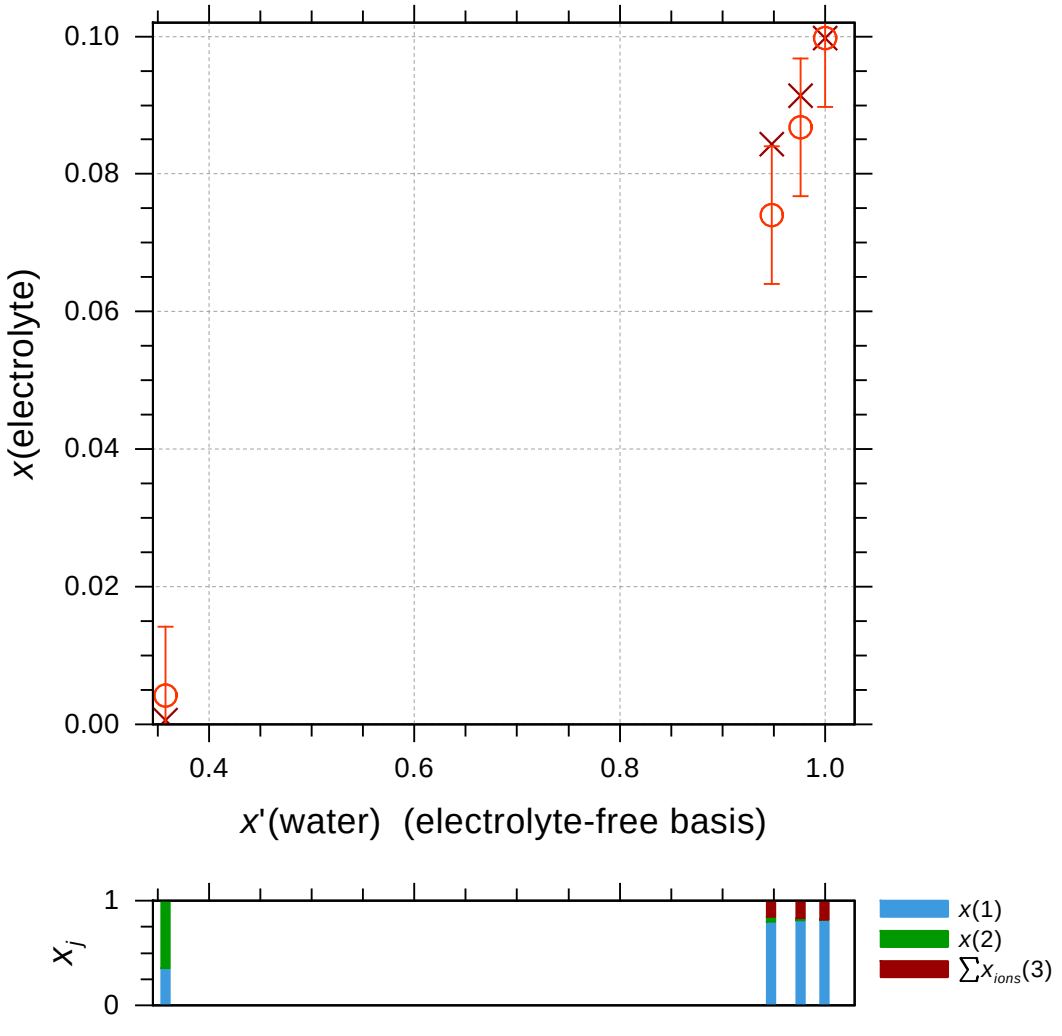


initial weighting of dataset:
w^{init}(0929) = 0.200
dataset contribution to F_{obj}:
fval(0929) = 5.2360E-02
rel. contribution = 0.0249 %

Fig. S0372 (AIOMFAC_output_0965)

H_2O (1) + 1,4-Dioxane (2) + NaCl (3)

Temperature: 298 K

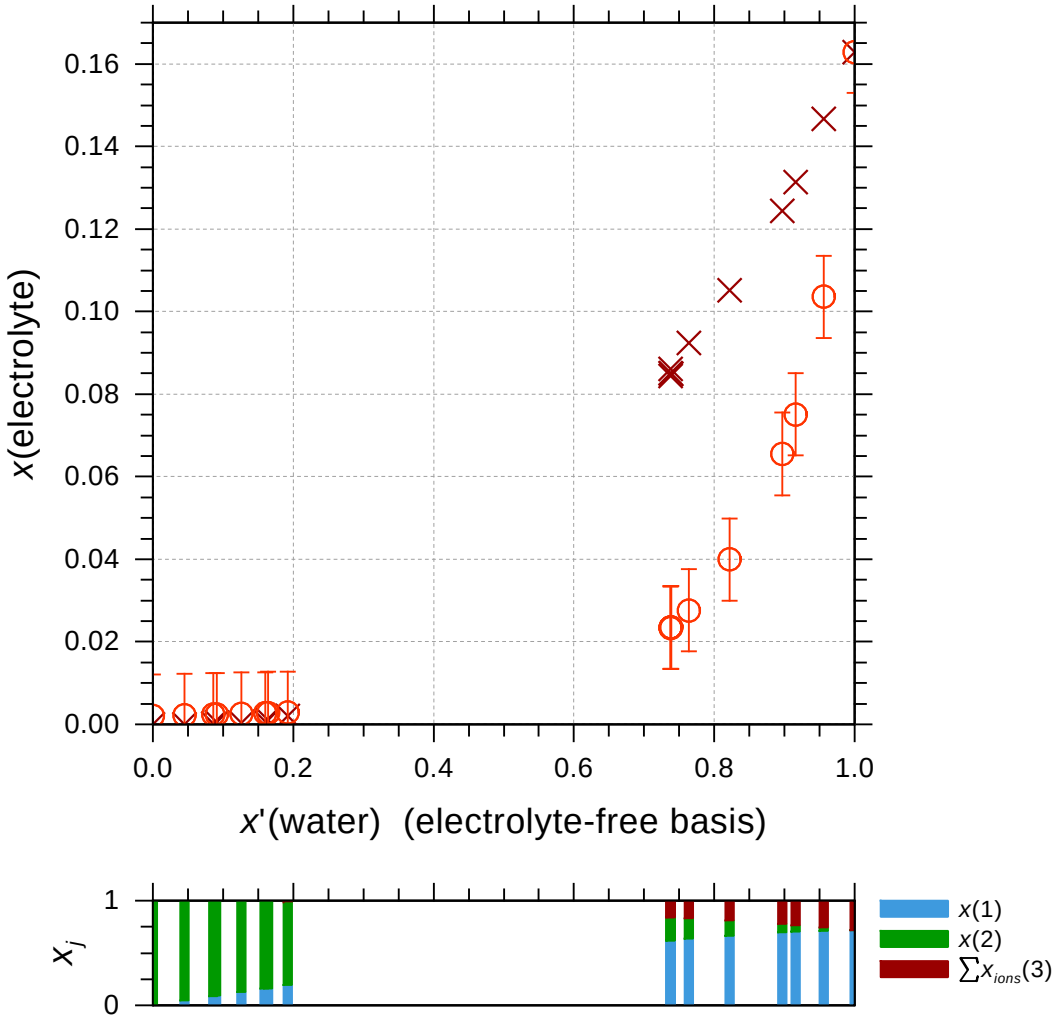


initial weighting of dataset:
w^{init}(0965) = 1.000
dataset contribution to F_{obj}:
fval(0965) = 1.2841E-01
rel. contribution = 0.0611 %

Fig. S0373 (AIOMFAC_output_0438)

H_2O (1) + 1,4-Dioxane (2) + $NaNO_3$ (3)

Temperature: 298 K

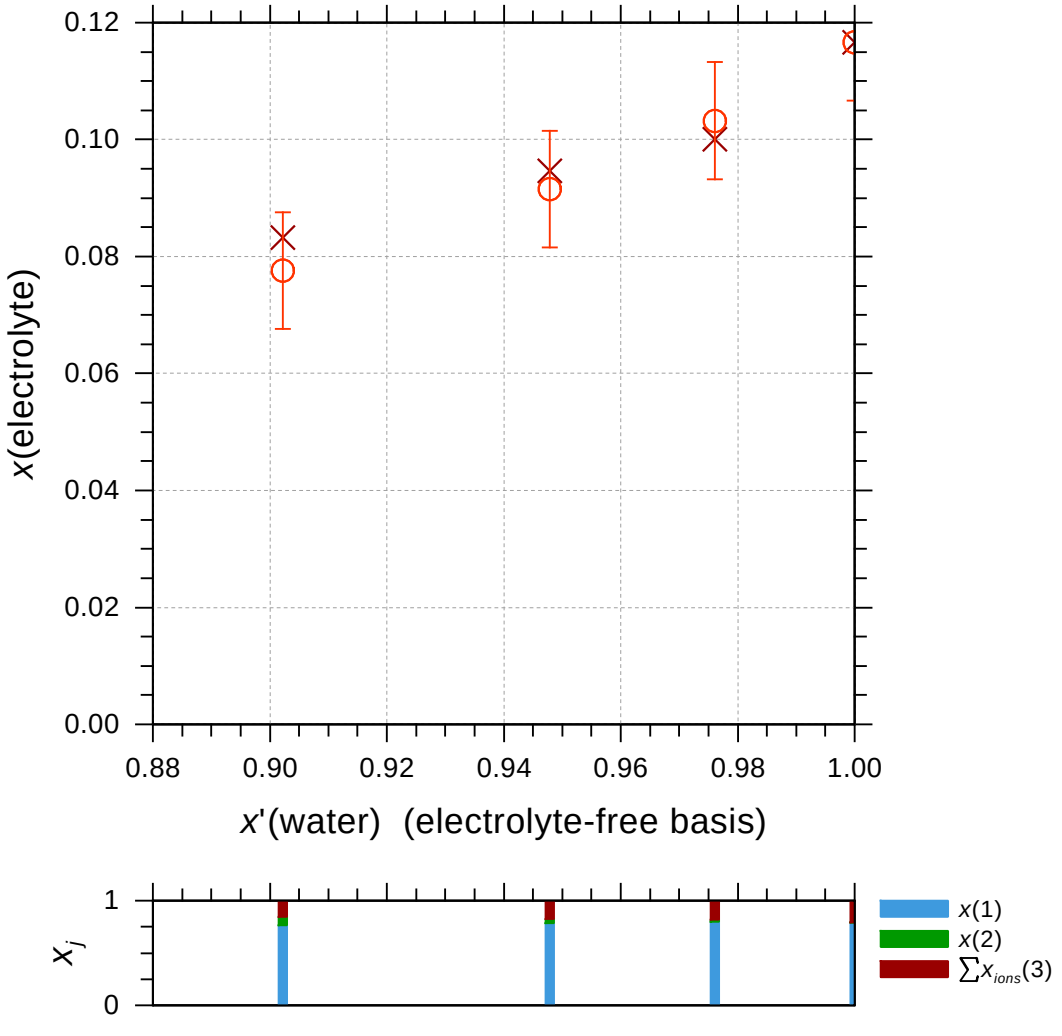


initial weighting of dataset:
$w^{init}(0438)$ = 1.000
dataset contribution to F_{obj}:
fval(0438) = 1.7662E+00
rel. contribution = 0.8399 %

Fig. S0374 (AIOMFAC_output_0964)

H_2O (1) + 1,4-Dioxane (2) + NH_4Cl (3)

Temperature: 298 K



initial weighting of dataset:
$w^{init}(0964)$ = 0.500
dataset contribution to F_{obj}:
fval(0964) = 2.7683E-03
rel. contribution = 0.0013 %

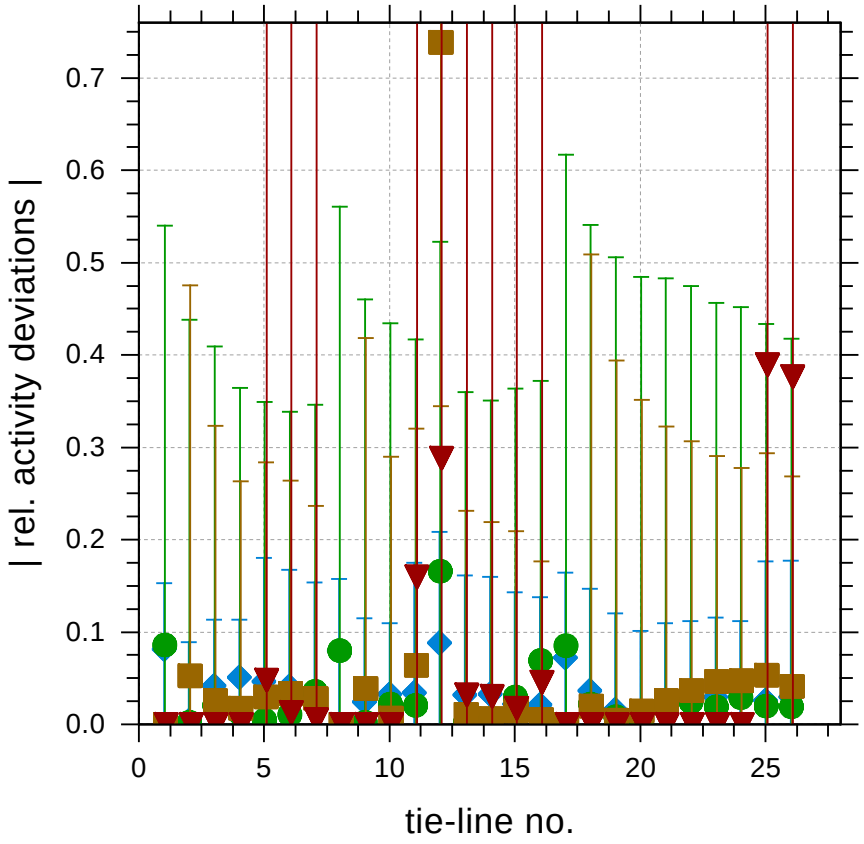
Fig. S0375 (AIOMFAC_output_0349)

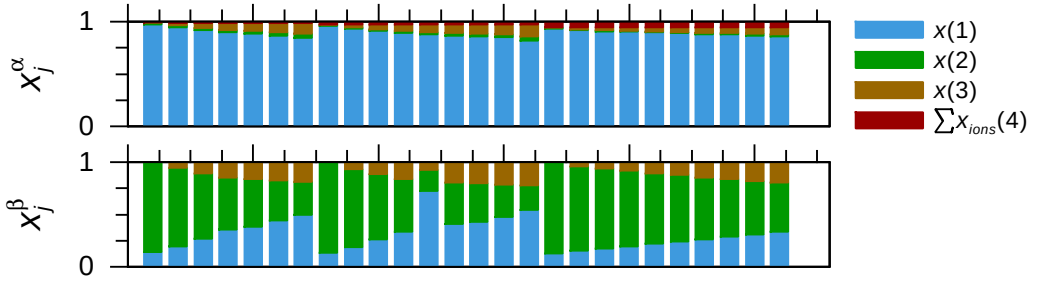
H_2O (1) + Ethyl_acetate (2) + Ethanol (3) + $CaCl_2$ (4)

Temperature: 298 K

left y-axis:

- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)



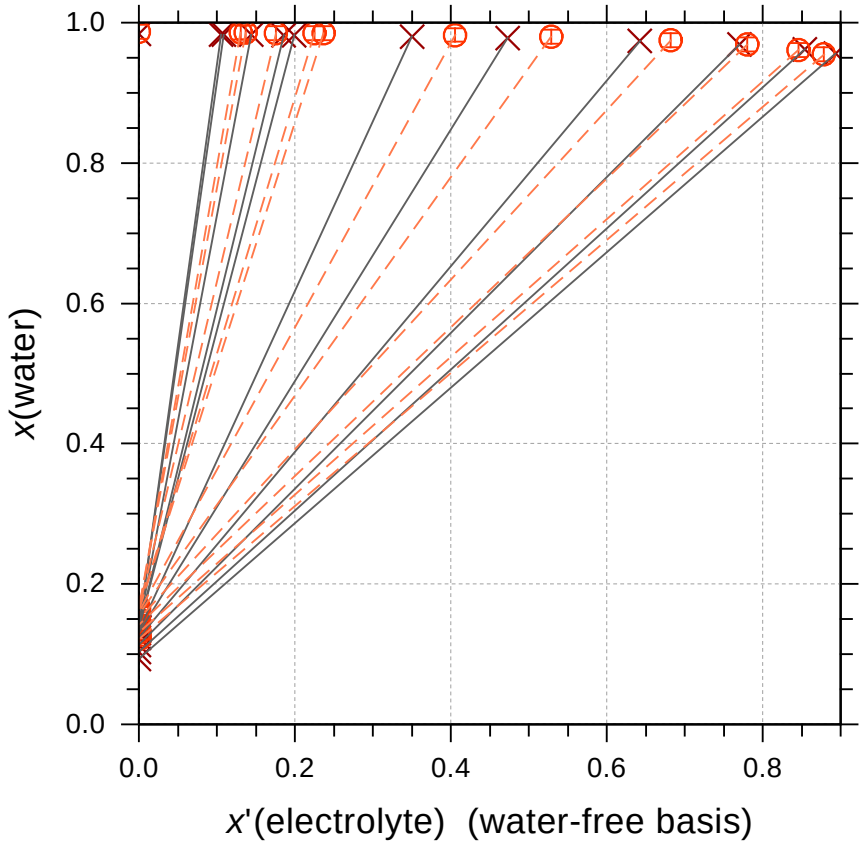


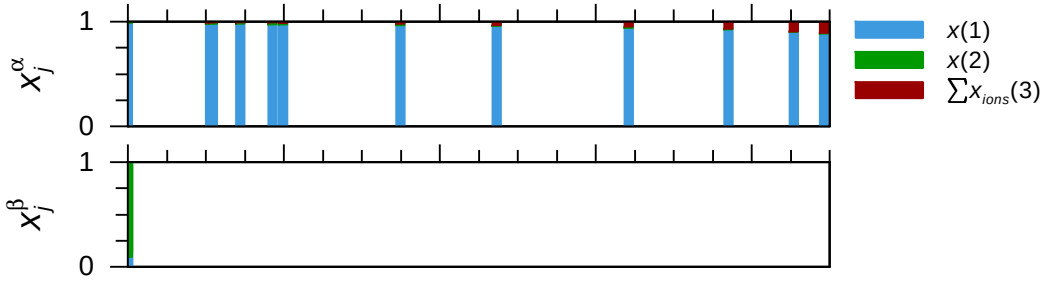
initial weighting of dataset:
$w^{init}(0349)$ = 1.000
dataset contribution to F_{obj}:
fval(0349) = 2.0900E-01
rel. contribution = 0.0994 %

Fig. S0376 (AIOMFAC_output_0350)

H_2O (1) + Ethyl_acetate (2) + $CaCl_2$ (3)

Temperature: 298 K





left y-axis:

× CaCl2+EthylAcetate+Water_LLE_Kumagae

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0350) = 1.000

dataset contribution to F_{obj}:

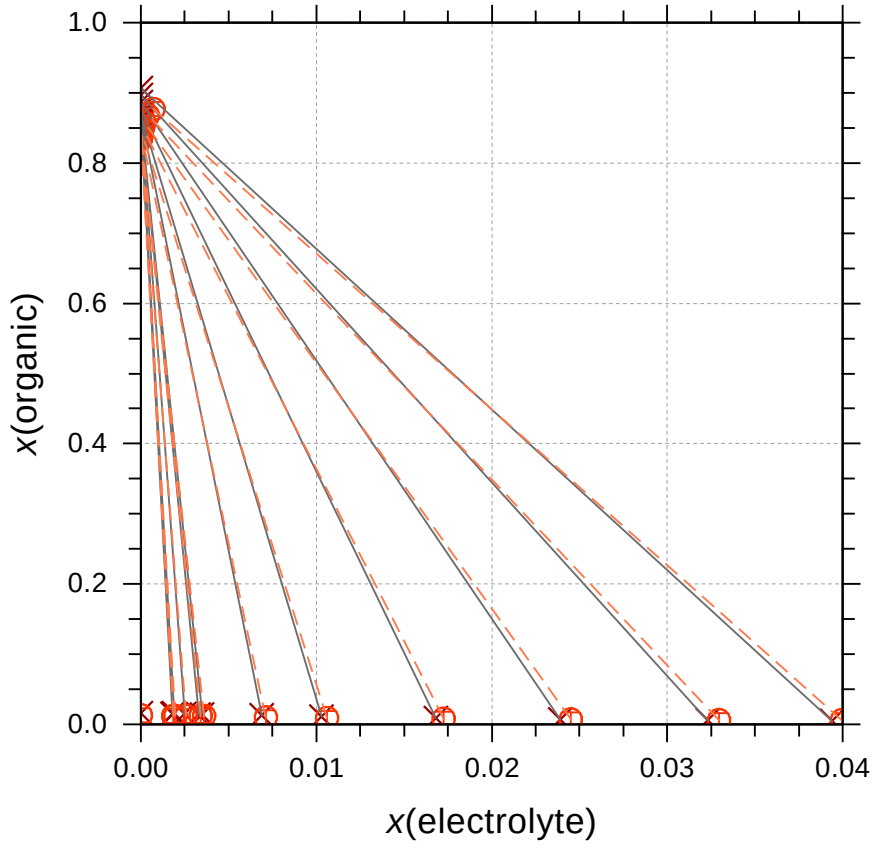
fval(0350) = 6.9120E-02

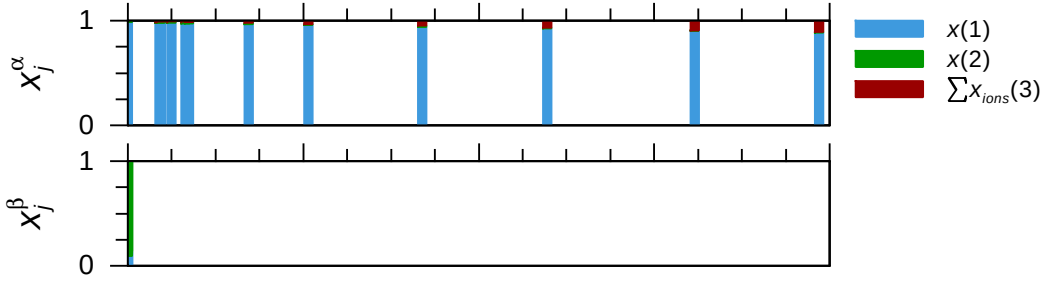
rel. contribution = 0.0329 %

Fig. S0376a (AIOMFAC_output_0350)

H_2O (1) + Ethyl_acetate (2) + $CaCl_2$ (3)

Temperature: 298 K





left y-axis:

× CaCl2+EthylAcetate+Water_LLE_Kumagae

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0350) = 1.000

dataset contribution to F_{obj}:

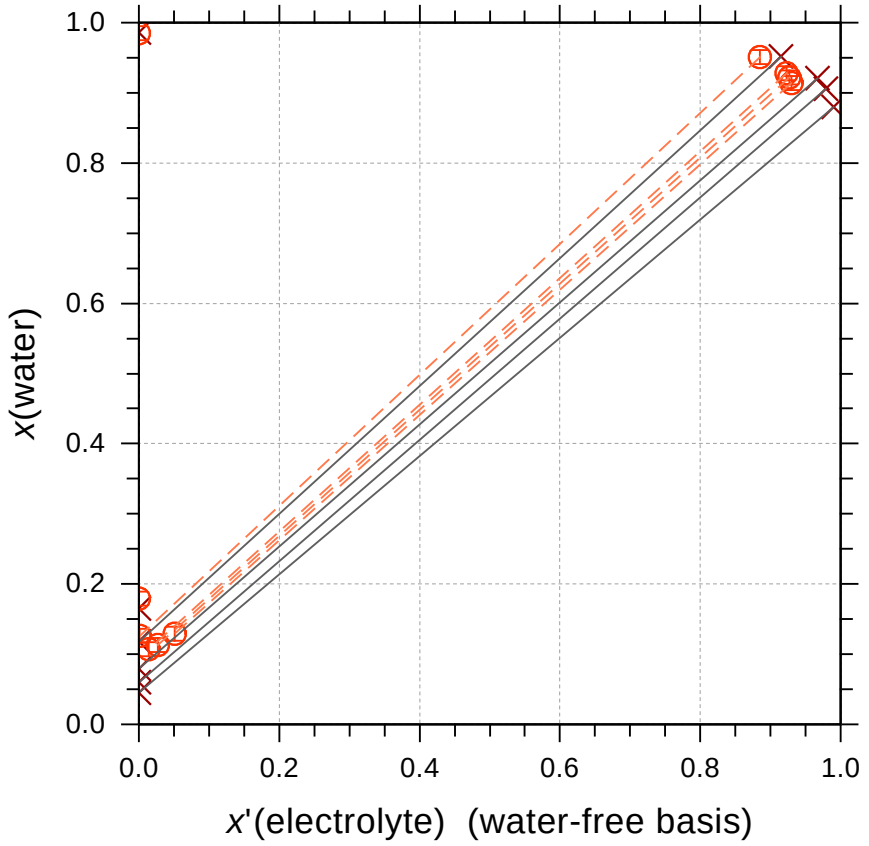
fval(0350) = 6.9120E-02

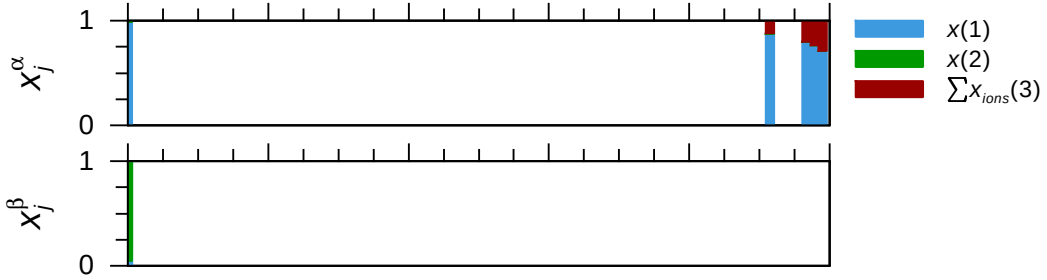
rel. contribution = 0.0329 %

Fig. S0377 (AIOMFAC_output_0434)

H_2O (1) + Ethyl_acetate (2) + $CaCl_2$ (3)

Temperature: 313 K





left y-axis:

× CaCl2+EthylAcetate+Water_LLE_Lin

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0434) = 0.800

dataset contribution to F_{obj}:

fval(0434) = 4.0264E-01

rel. contribution = 0.1915 %

Fig. S0377a (AIOMFAC_output_0434)

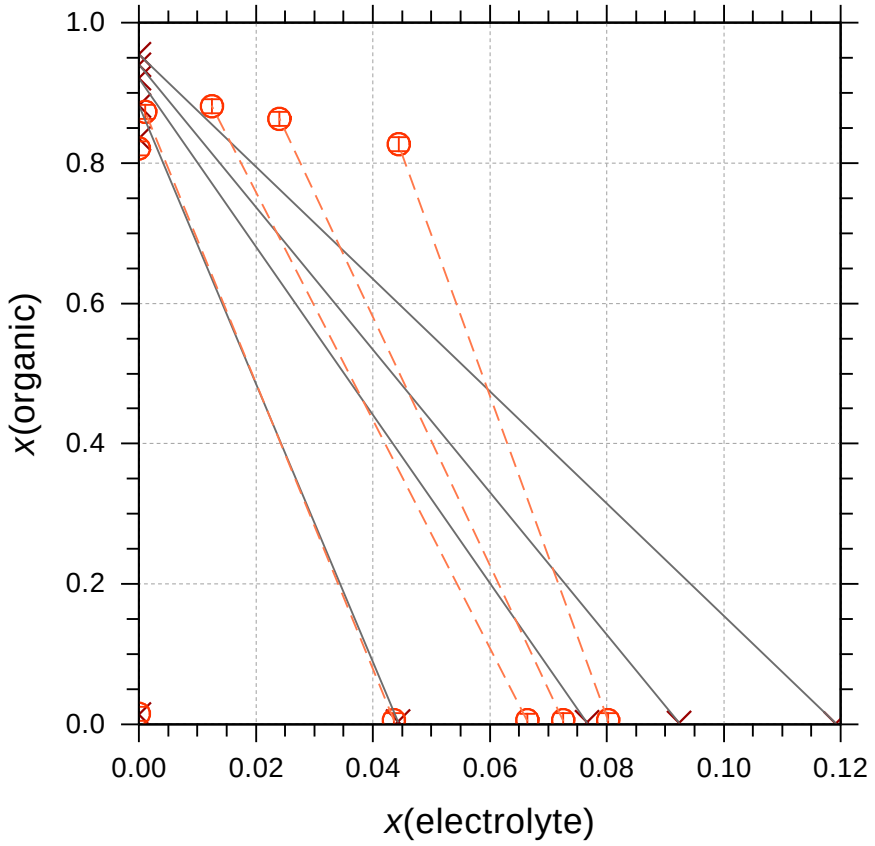
H_2O (1) + Ethyl_acetate (2) + $CaCl_2$ (3)

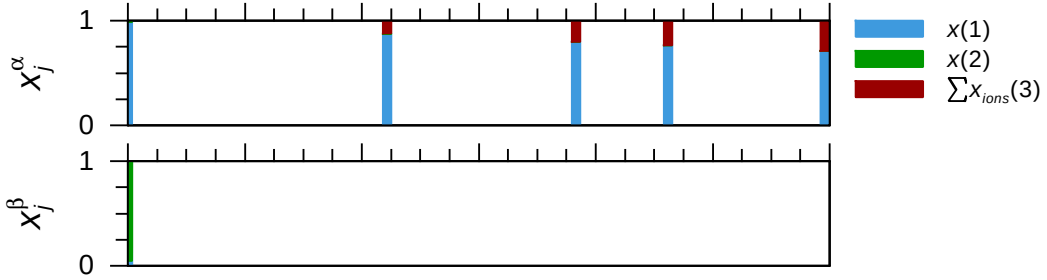
Temperature: 313 K

left y-axis:

× CaCl2+EthylAcetate+Water_LLE_Lin

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0434) = 0.800

dataset contribution to F_{obj}:

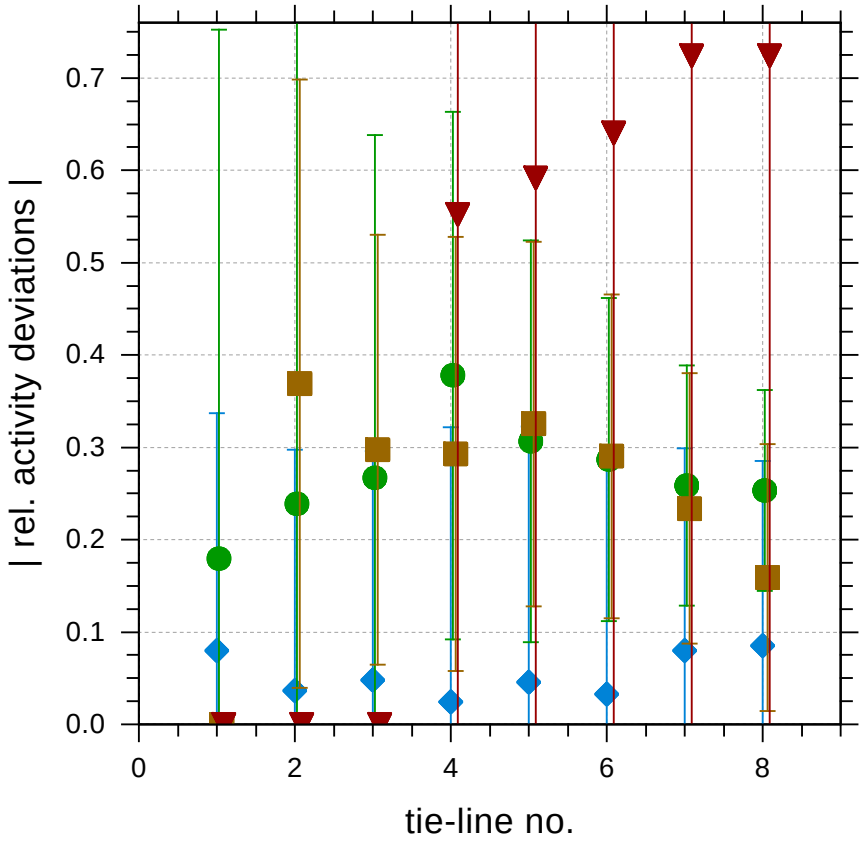
fval(0434) = 4.0264E-01

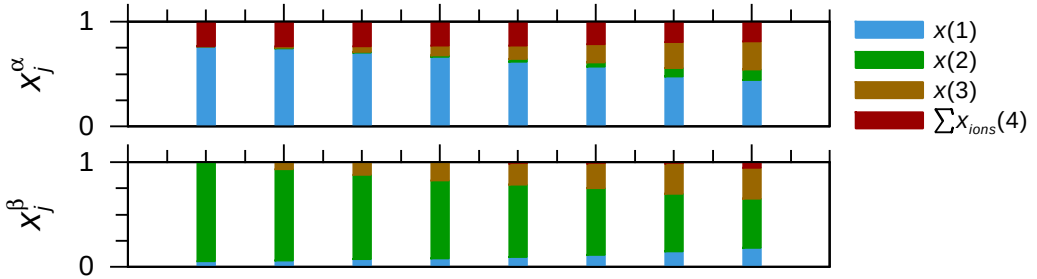
rel. contribution = 0.1915 %

Fig. S0378 (AIOMFAC_output_0435)

H_2O (1) + Ethyl_acetate (2) + Ethanol (3) + $CaCl_2$ (4)

Temperature: 283 K





left y-axis:

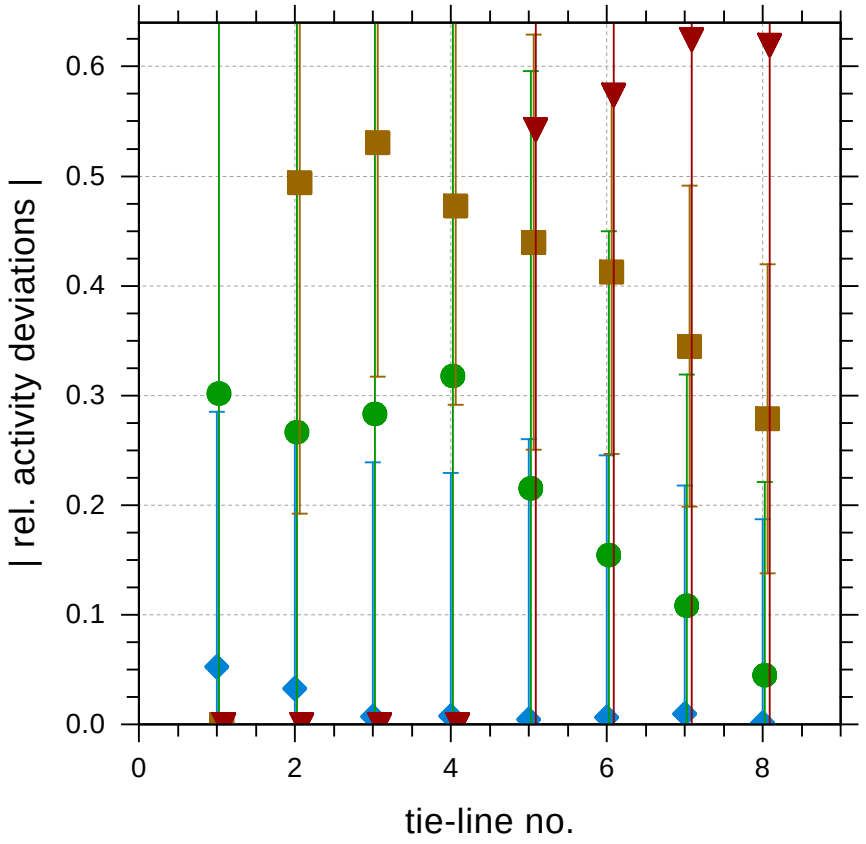
- AIOMFAC water (1) activity, rel. deviations
- AIOMFAC organic (2) activity, rel. deviations
- AIOMFAC organic (3) activity, rel. deviations
- AIOMFAC IAP, rel. deviations comp.(4)

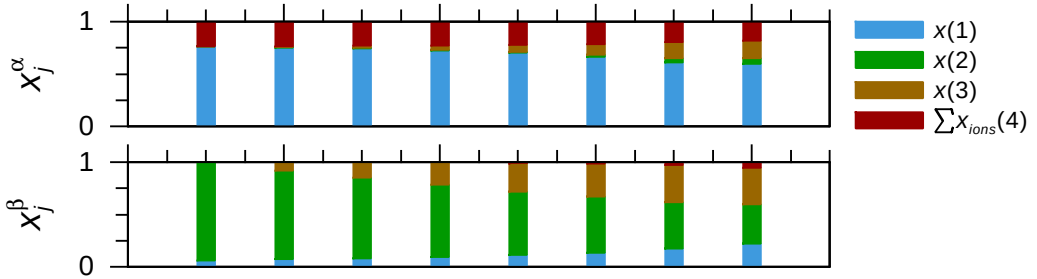
initial weighting of dataset:
$w^{init}(0435)$ = 0.800
dataset contribution to F_{obj}:
fval(0435) = 1.6673E+00
rel. contribution = 0.7929 %

Fig. S0379 (AIOMFAC_output_0436)

H_2O (1) + Ethyl_acetate (2) + Ethanol (3) + $CaCl_2$ (4)

Temperature: 313 K



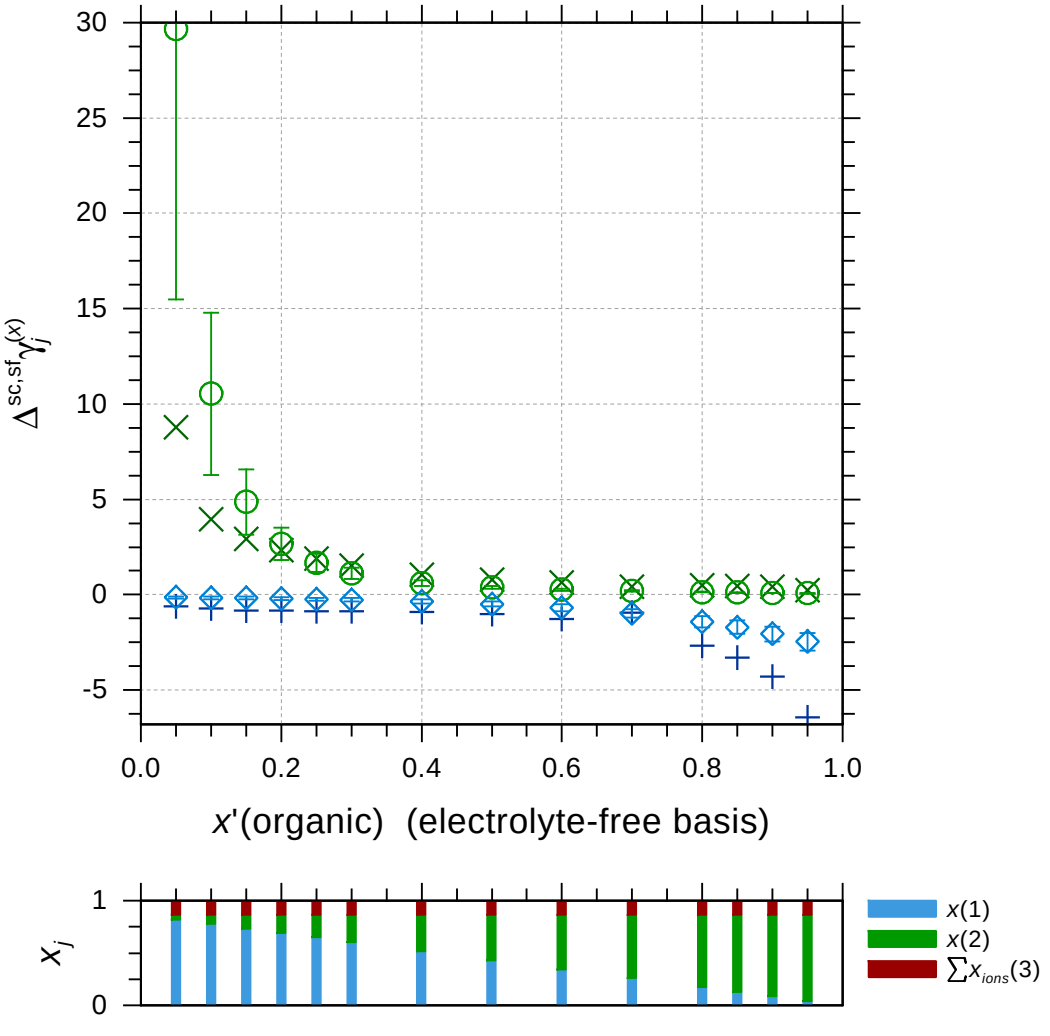


initial weighting of dataset:
$w^{init}(0436)$ = 0.800
dataset contribution to F_{obj}:
fval(0436) = 1.5691E+00
rel. contribution = 0.7462 %

Fig. S0380 (AIOMFAC_output_0915)

H_2O (1) + Ethyl_acetate (2) + $CaCl_2$ (3)

Temperature range: 344 -- 349 K



initial weighting of dataset:

w^{init}(0915) = 0.500

dataset contribution to F_{obj}:

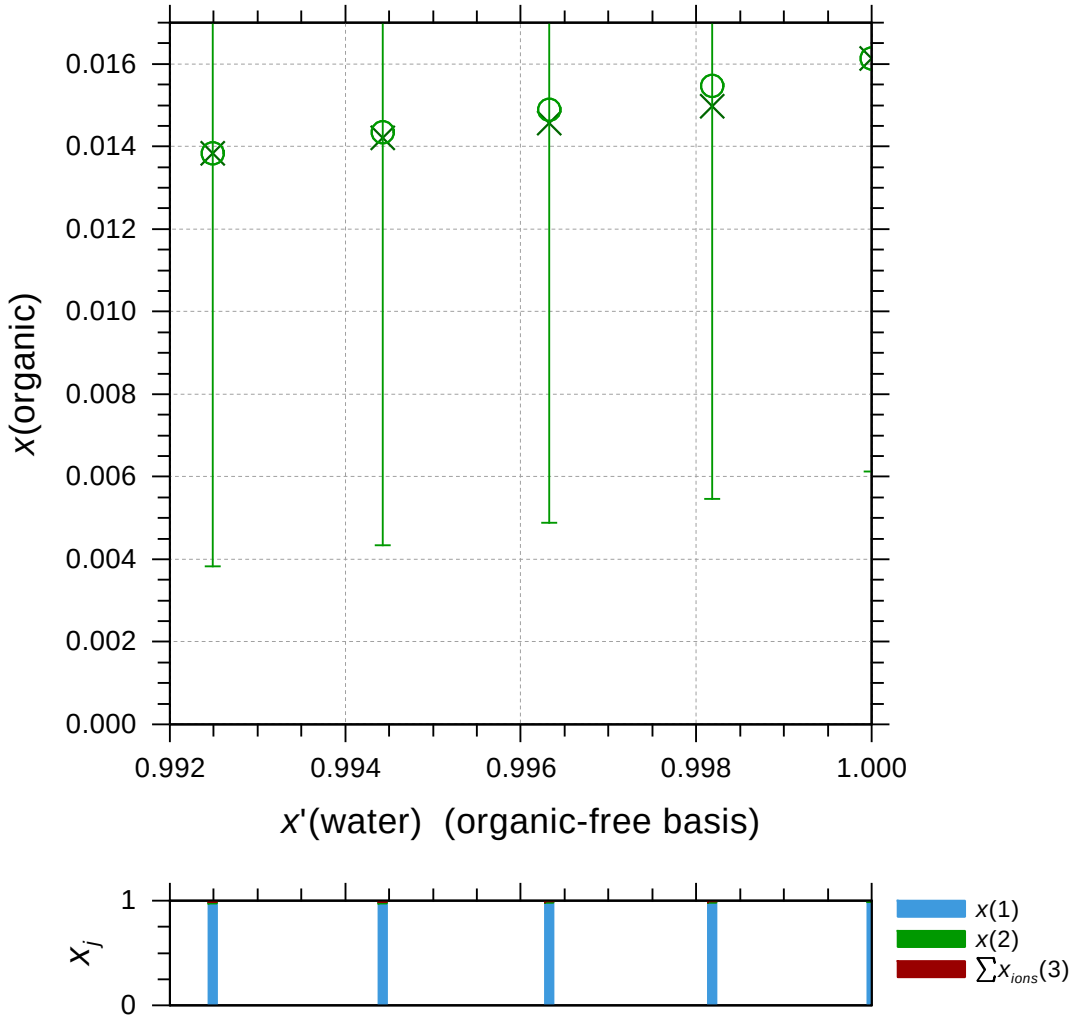
fval(0915) = 1.1368E+00

rel. contribution = 0.5406 %

Fig. S0381 (AIOMFAC_output_0433)

H_2O (1) + Ethyl_acetate (2) + KBr (3)

Temperature: 303 K

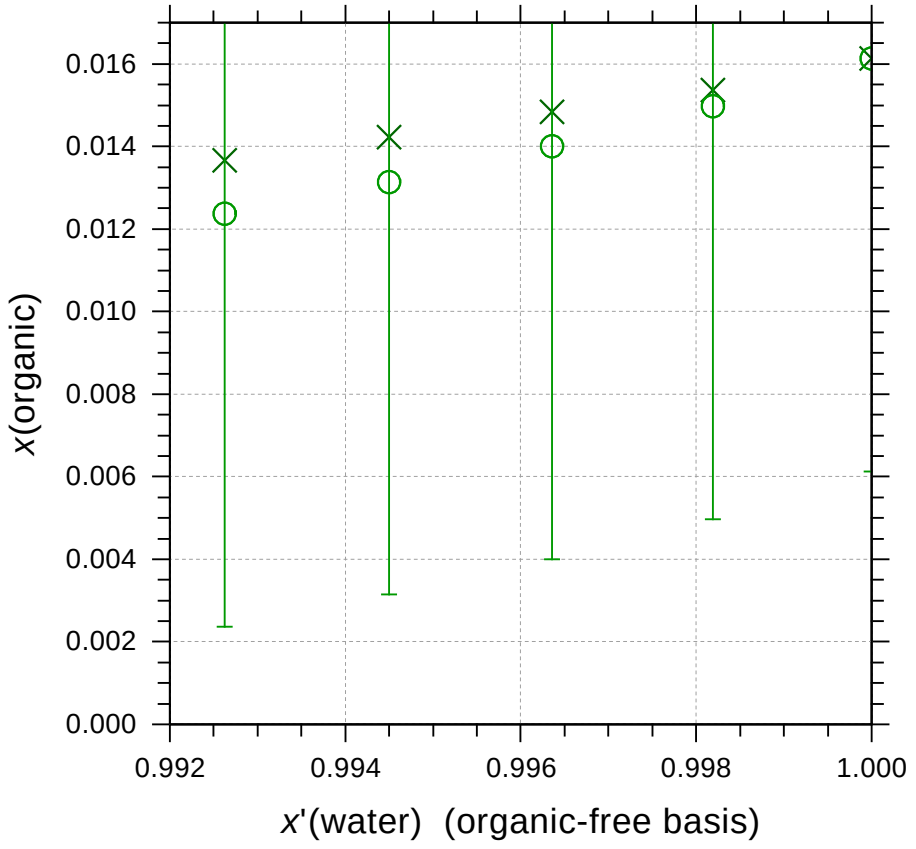


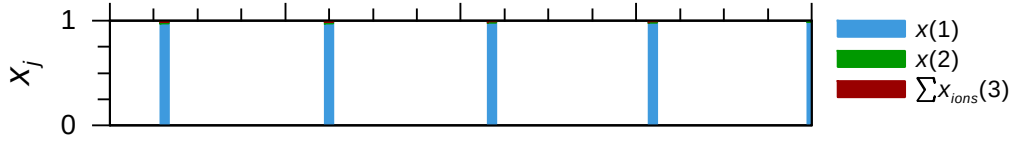
initial weighting of dataset:
$w^{init}(0433)$ = 1.000
dataset contribution to F_{obj}:
fval(0433) = 5.8974E-04
rel. contribution = 0.0003 %

Fig. S0382 (AIOMFAC_output_0432)

H_2O (1) + Ethyl_acetate (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl+EthylAcetate+Water_SLE_Altshuller

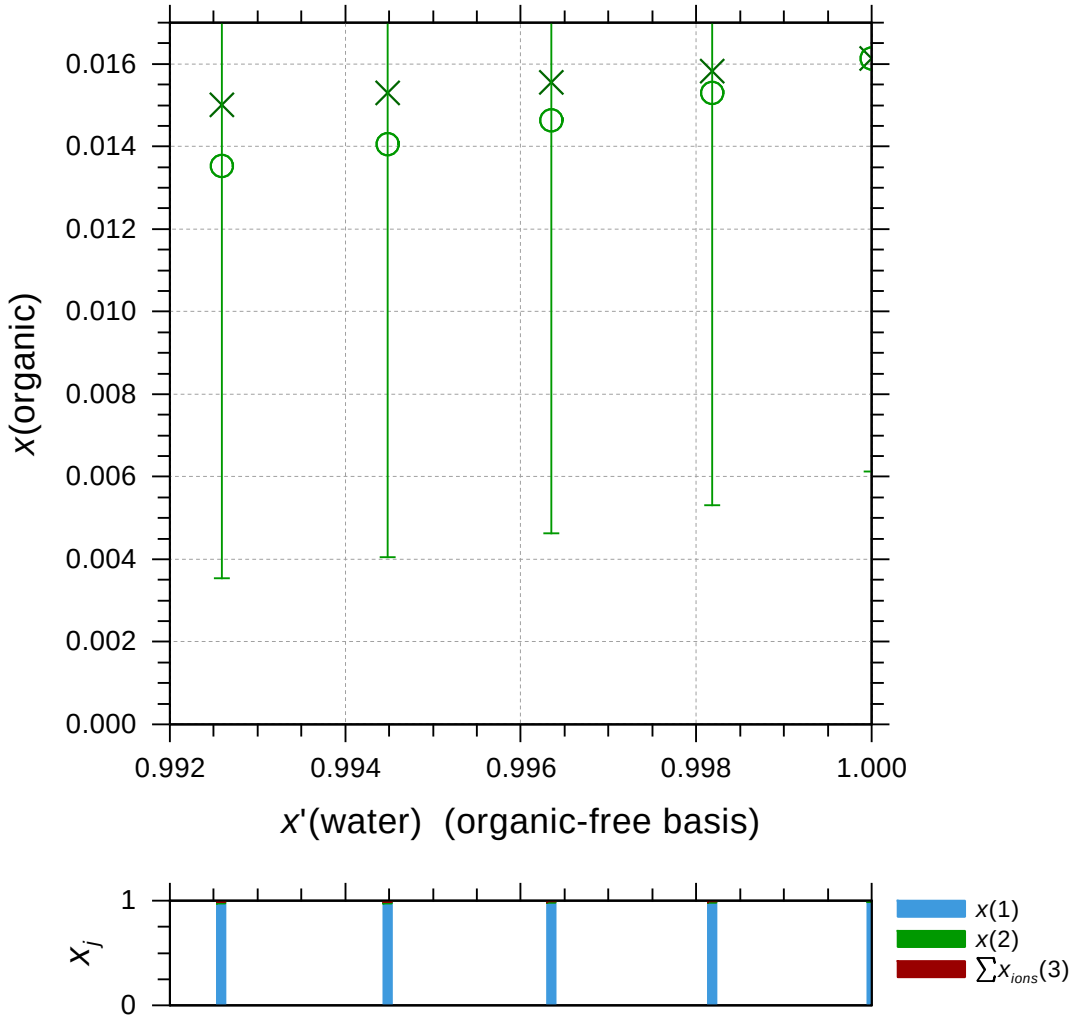
○ AIOMFAC calc. SLE composition

initial weighting of dataset:
w^{init}(0432) = 1.000
dataset contribution to F_{obj}:
fval(0432) = 6.4225E-03
rel. contribution = 0.0031 %

Fig. S0383 (AIOMFAC_output_0429)

H_2O (1) + Ethyl_acetate (2) + LiBr (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0429)$ = 1.000

dataset contribution to F_{obj}:

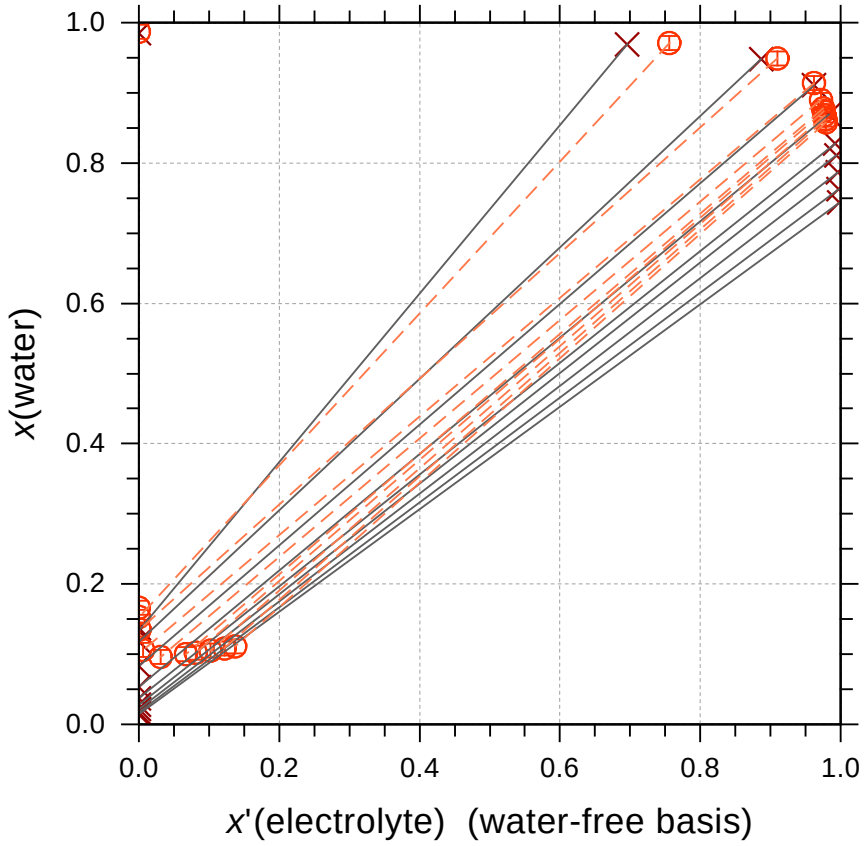
fval(0429) = 7.6053E-03

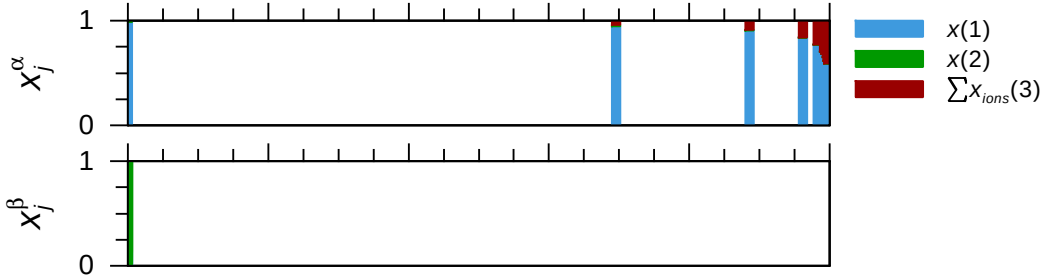
rel. contribution = 0.0036 %

Fig. S0384 (AIOMFAC_output_0347)

H_2O (1) + Ethyl_acetate (2) + LiCl (3)

Temperature: 298 K





left y-axis:

× LiCl+EthylAcetate+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0347) = 1.000

dataset contribution to F_{obj}:

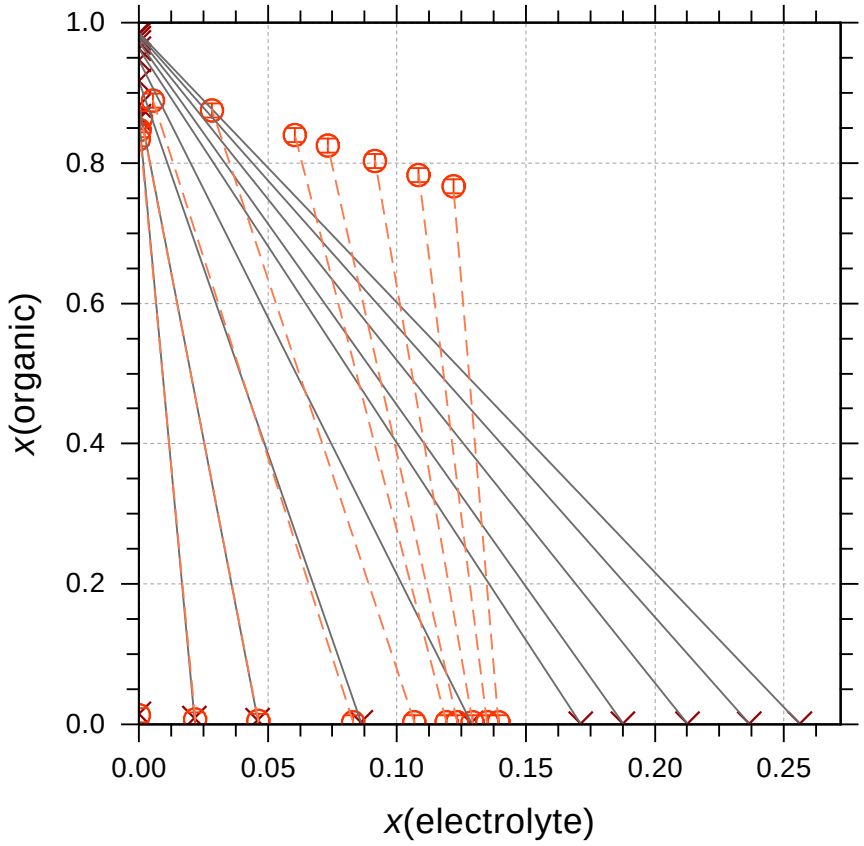
fval(0347) = 9.6541E+00

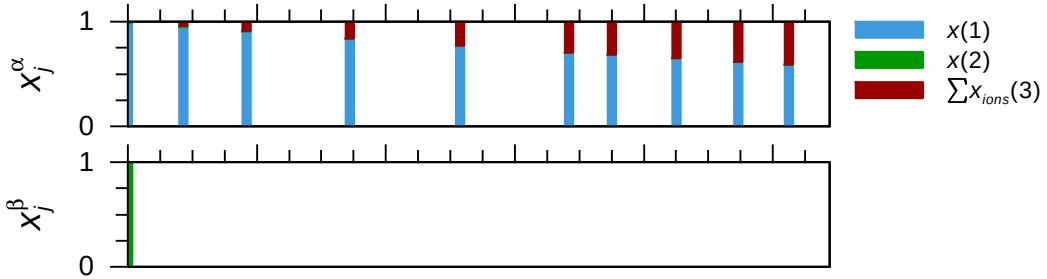
rel. contribution = 4.5908 %

Fig. S0384a (AIOMFAC_output_0347)

H_2O (1) + Ethyl_acetate (2) + LiCl (3)

Temperature: 298 K





left y-axis:

× LiCl+EthylAcetate+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0347) = 1.000

dataset contribution to F_{obj}:

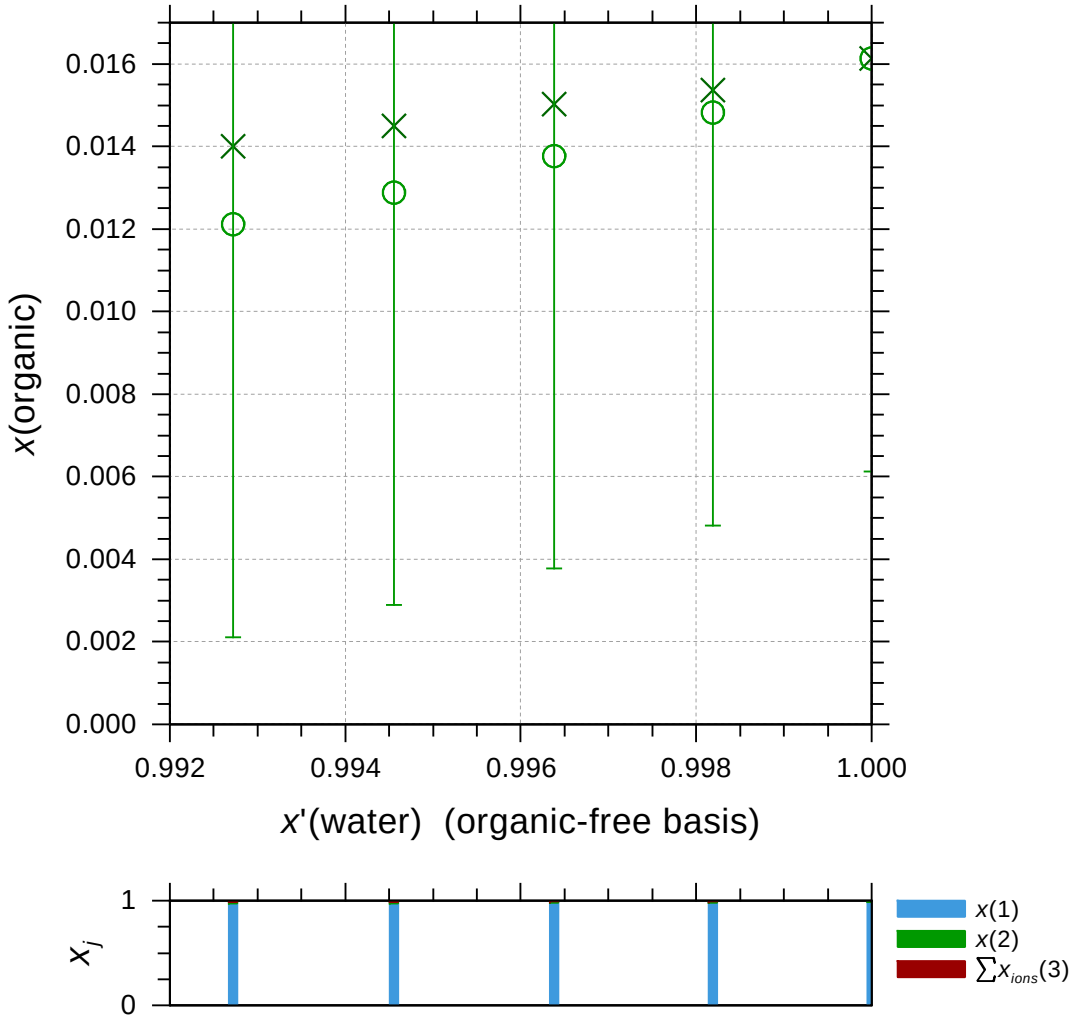
fval(0347) = 9.6541E+00

rel. contribution = 4.5908 %

Fig. S0385 (AIOMFAC_output_0428)

H_2O (1) + Ethyl_acetate (2) + LiCl (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0428)$ = 1.000

dataset contribution to F_{obj}:

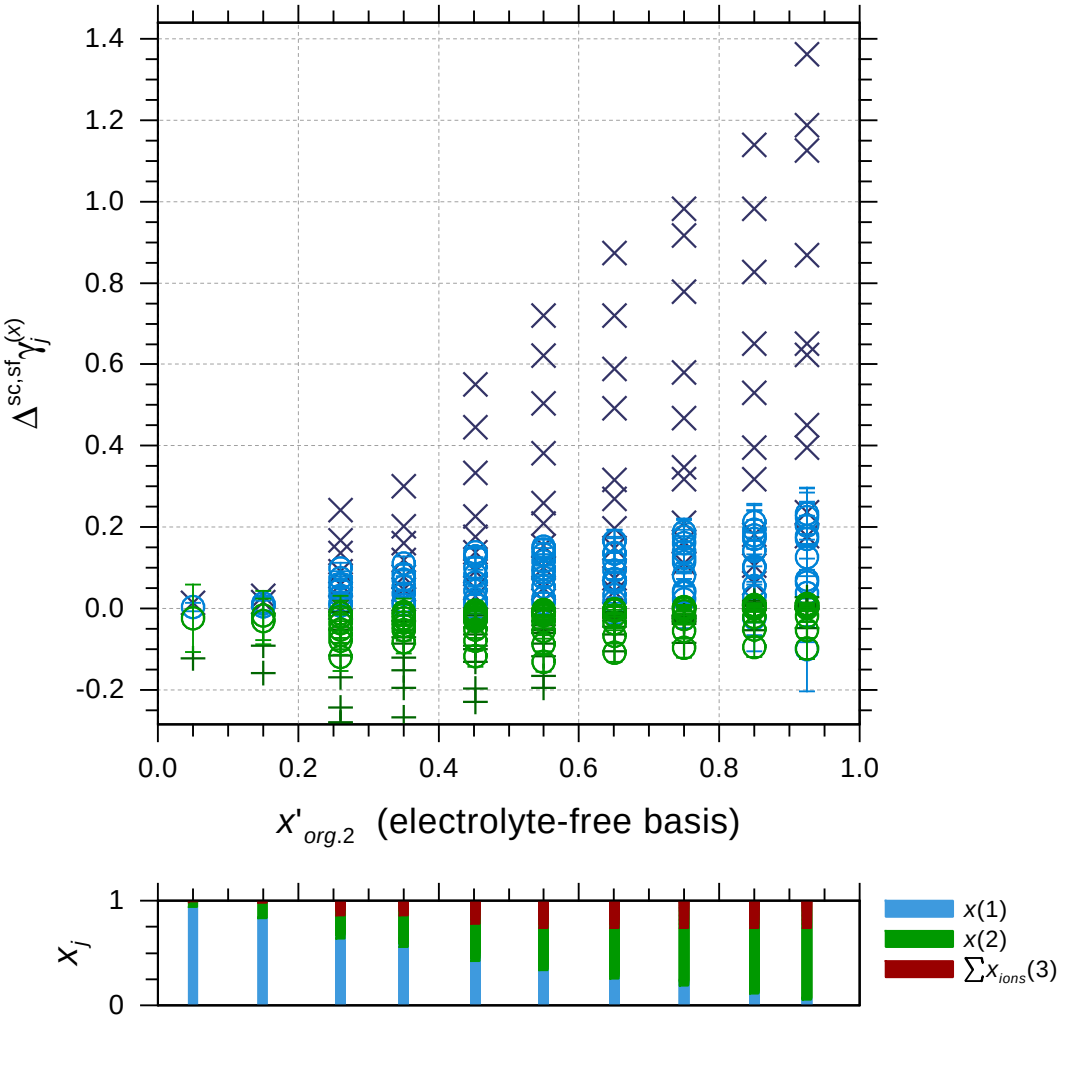
fval(0428) = 1.3476E-02

rel. contribution = 0.0064 %

Fig. S0386 (AIOMFAC_output_0935)

Ethyl_acetate (1) + Ethanol (2) + $LiNO_3$ (3)

Temperature range: 345 -- 356 K



initial weighting of dataset:

$w^{init}(0935)$ = 0.500

dataset contribution to F_{obj}:

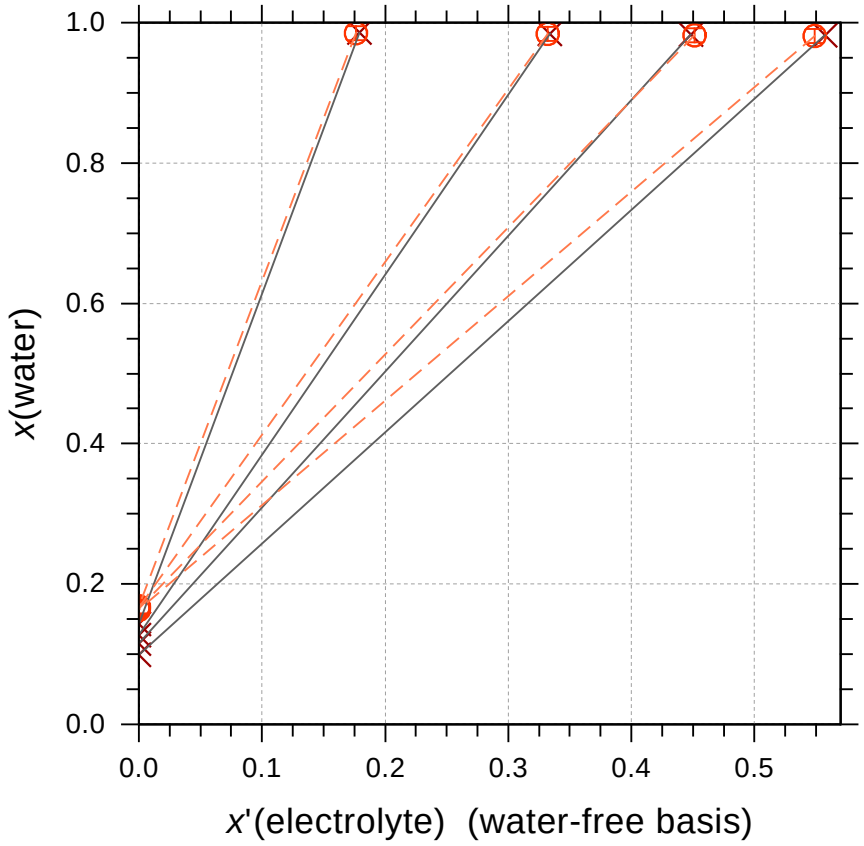
fval(0935) = 2.4380E-01

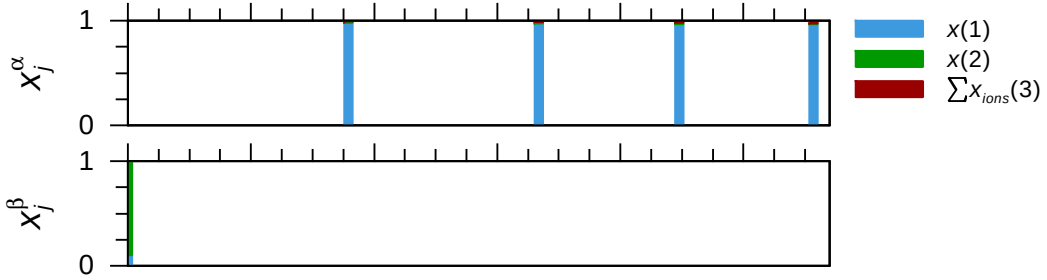
rel. contribution = 0.1159 %

Fig. S0387 (AIOMFAC_output_0437)

H_2O (1) + Ethyl_acetate (2) + Na_2SO_4 (3)

Temperature: 303 K





left y-axis:

× Na2SO4+EthylAcetate+Water_LLE_Nakamura

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0437) = 1.000

dataset contribution to F_{obj}:

fval(0437) = 1.2505E-01

rel. contribution = 0.0595 %

Fig. S0387a (AIOMFAC_output_0437)

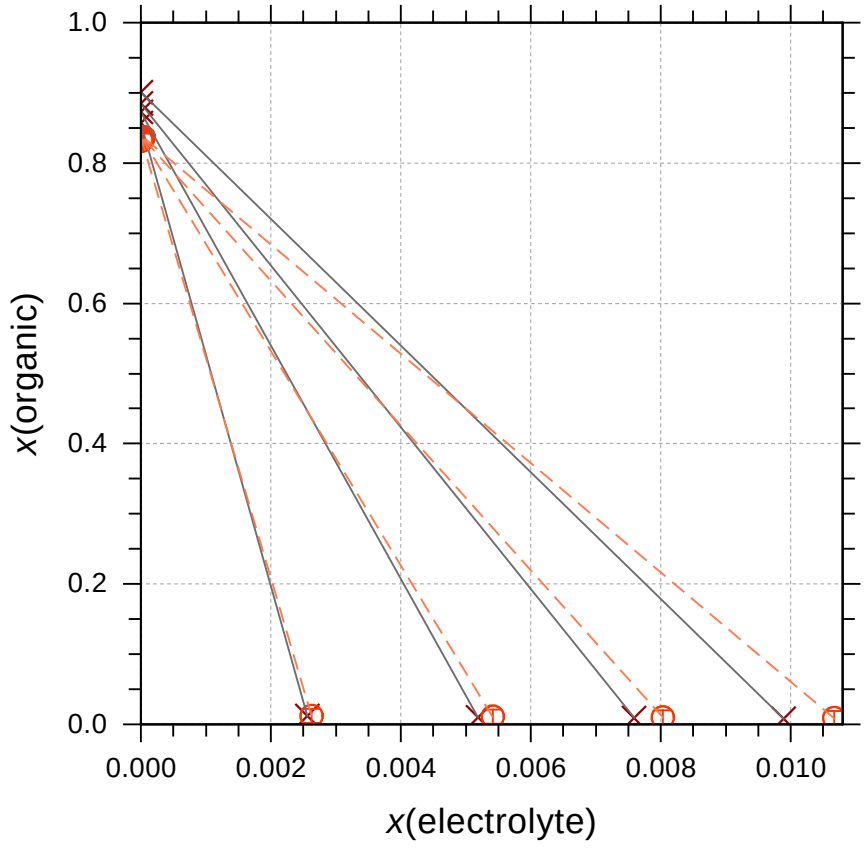
H_2O (1) + Ethyl_acetate (2) + Na_2SO_4 (3)

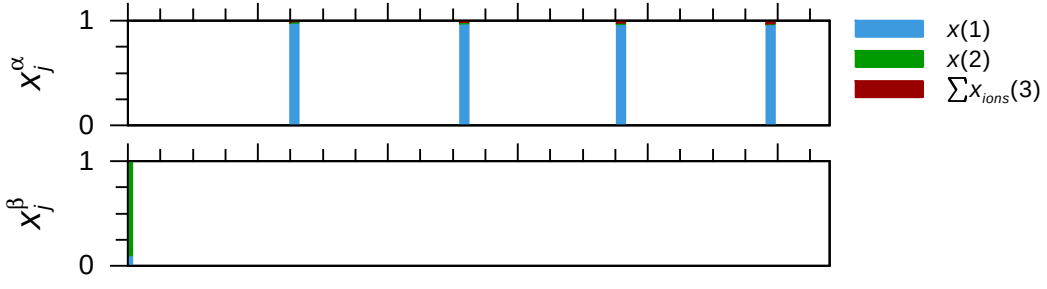
Temperature: 303 K

left y-axis:

× Na2SO4+EthylAcetate+Water_LLE_Nakamura

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0437) = 1.000

dataset contribution to F_{obj}:

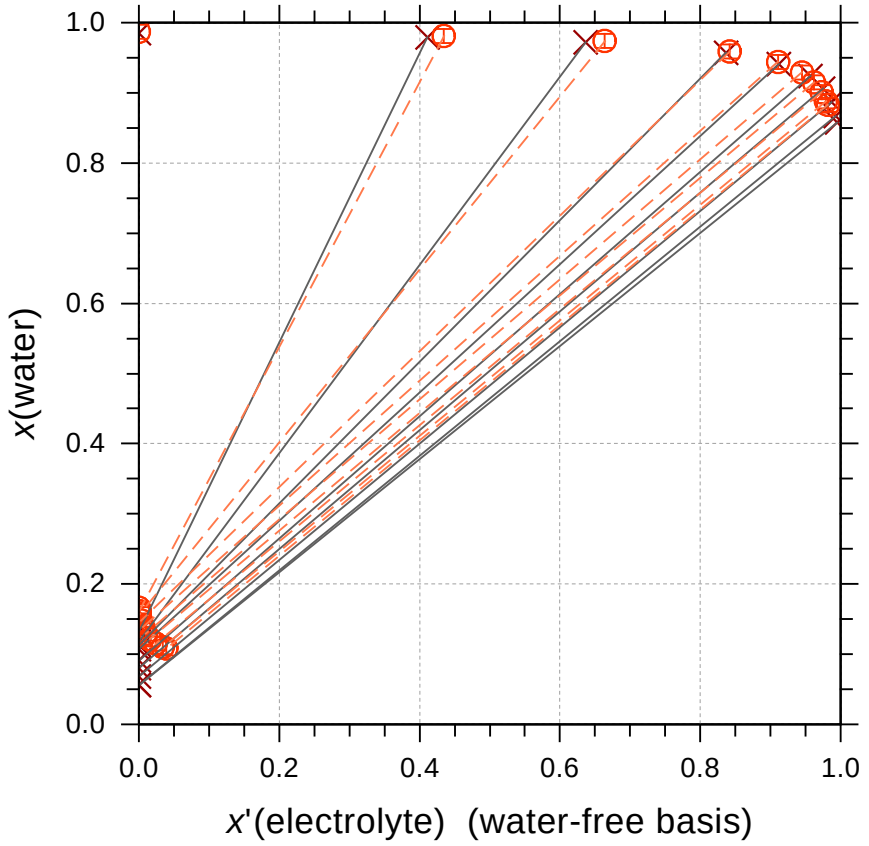
fval(0437) = 1.2505E-01

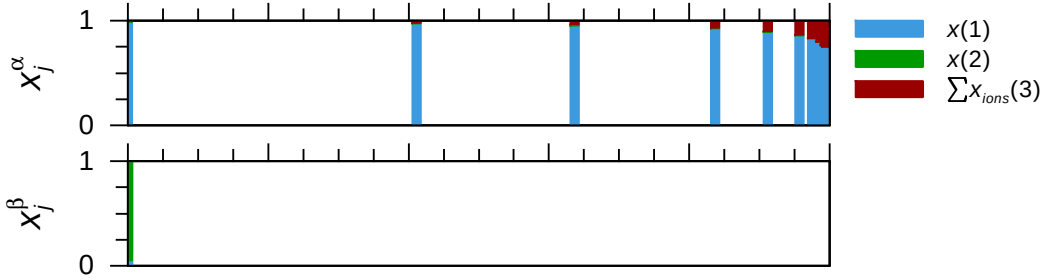
rel. contribution = 0.0595 %

Fig. S0388 (AIOMFAC_output_0346)

H_2O (1) + Ethyl_acetate (2) + NaBr (3)

Temperature: 298 K





left y-axis:

× NaBr+EthylAcetate+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0346) = 1.000

dataset contribution to F_{obj}:

fval(0346) = 1.2200E+01

rel. contribution = 5.8014 %

Fig. S0388a (AIOMFAC_output_0346)

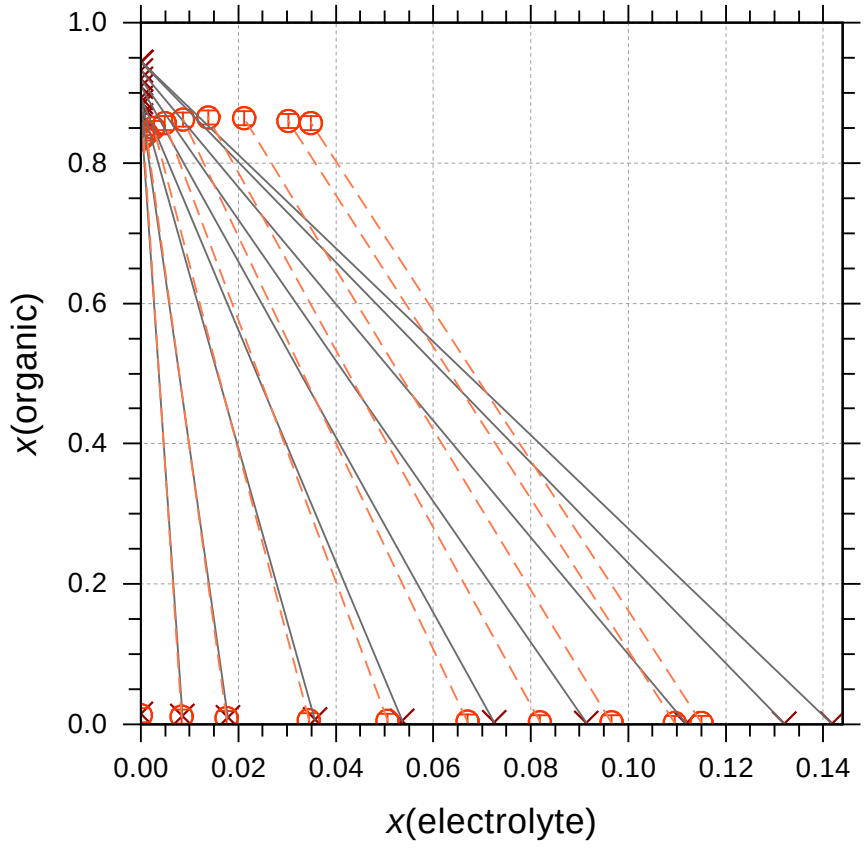
H_2O (1) + Ethyl_acetate (2) + NaBr (3)

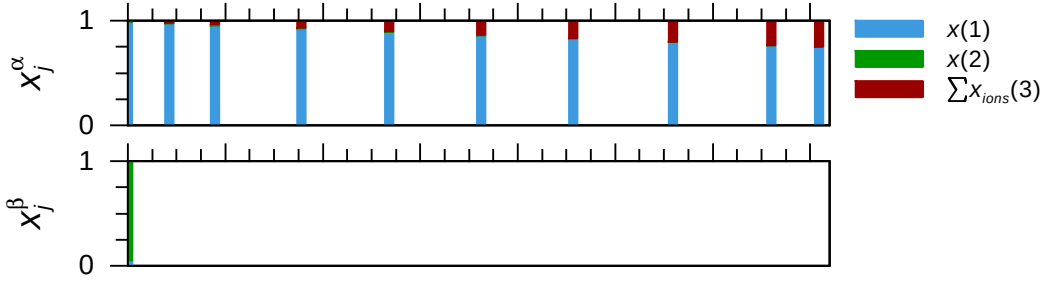
Temperature: 298 K

left y-axis:

× NaBr+EthylAcetate+Water_LLE_Al-Sahhaf

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0346) = 1.000

dataset contribution to F_{obj}:

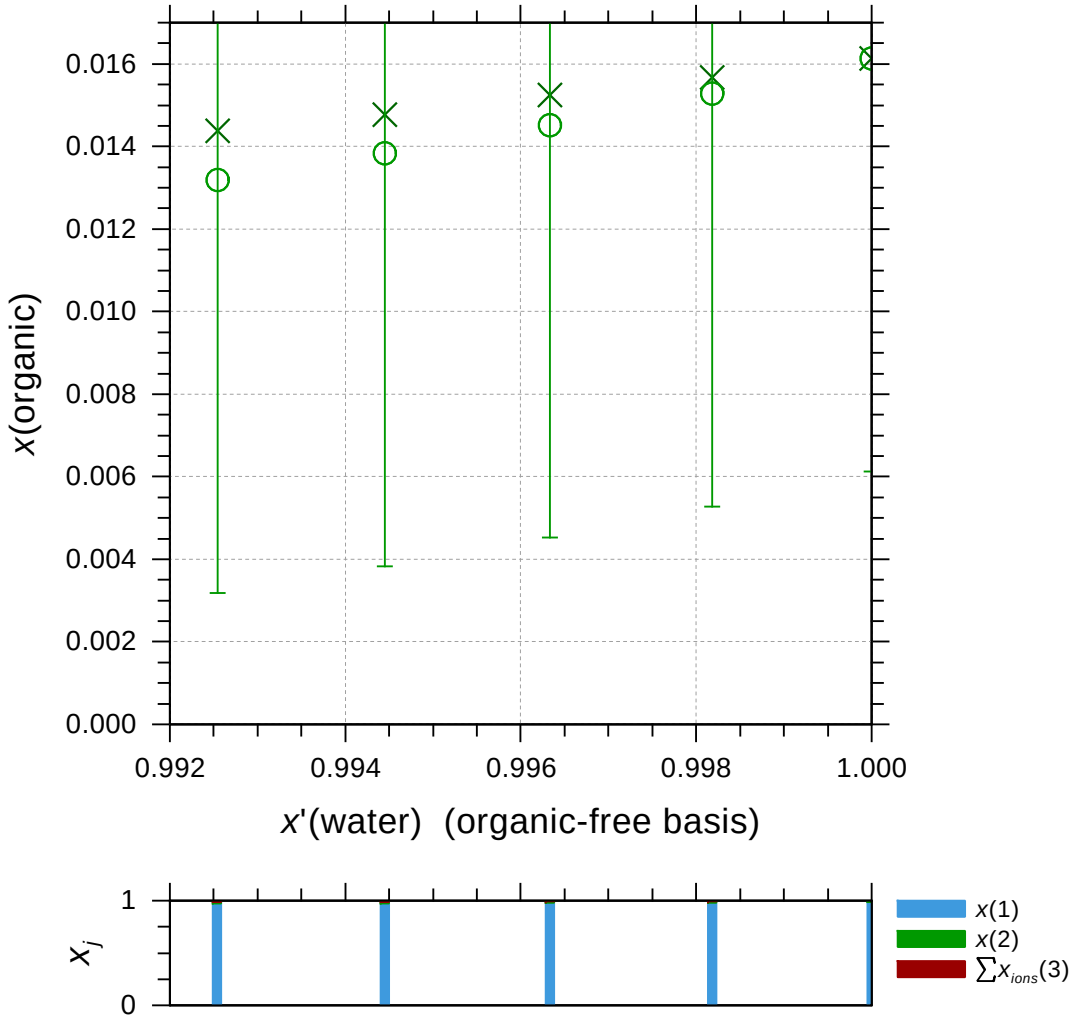
fval(0346) = 1.2200E+01

rel. contribution = 5.8014 %

Fig. S0389 (AIOMFAC_output_0431)

H_2O (1) + Ethyl_acetate (2) + NaBr (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0431)$ = 1.000

dataset contribution to F_{obj}:

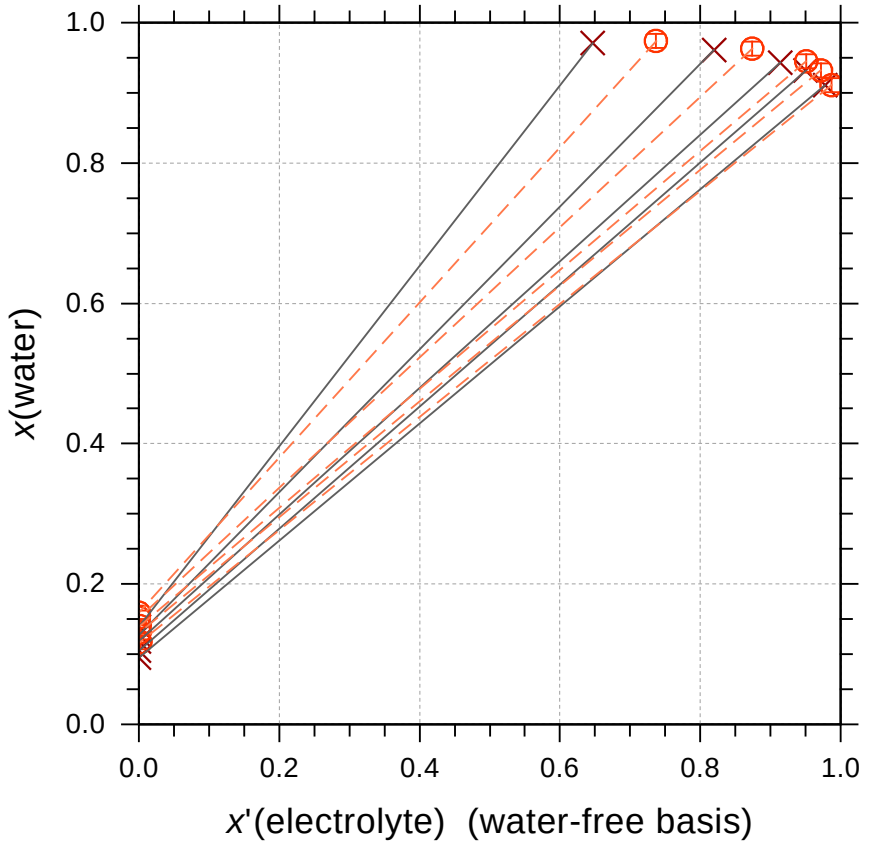
fval(0431) = 4.8906E-03

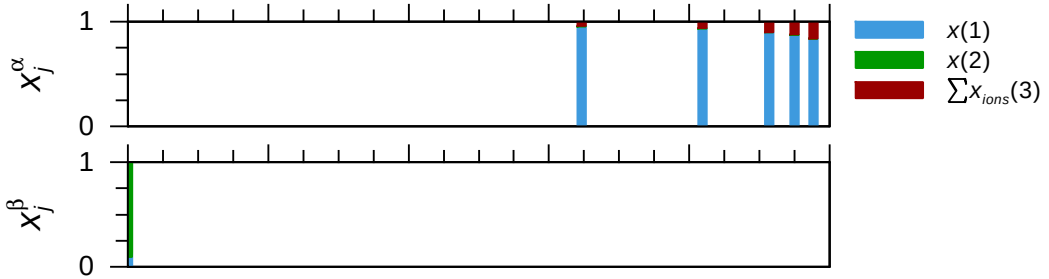
rel. contribution = 0.0023 %

Fig. S0390 (AIOMFAC_output_0348)

H_2O (1) + Ethyl_acetate (2) + NaCl (3)

Temperature: 303 K





left y-axis:

× NaCl+EthylAcetate+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0348) = 1.000

dataset contribution to F_{obj}:

fval(0348) = 7.2358E+00

rel. contribution = 3.4409 %

Fig. S0390a (AIOMFAC_output_0348)

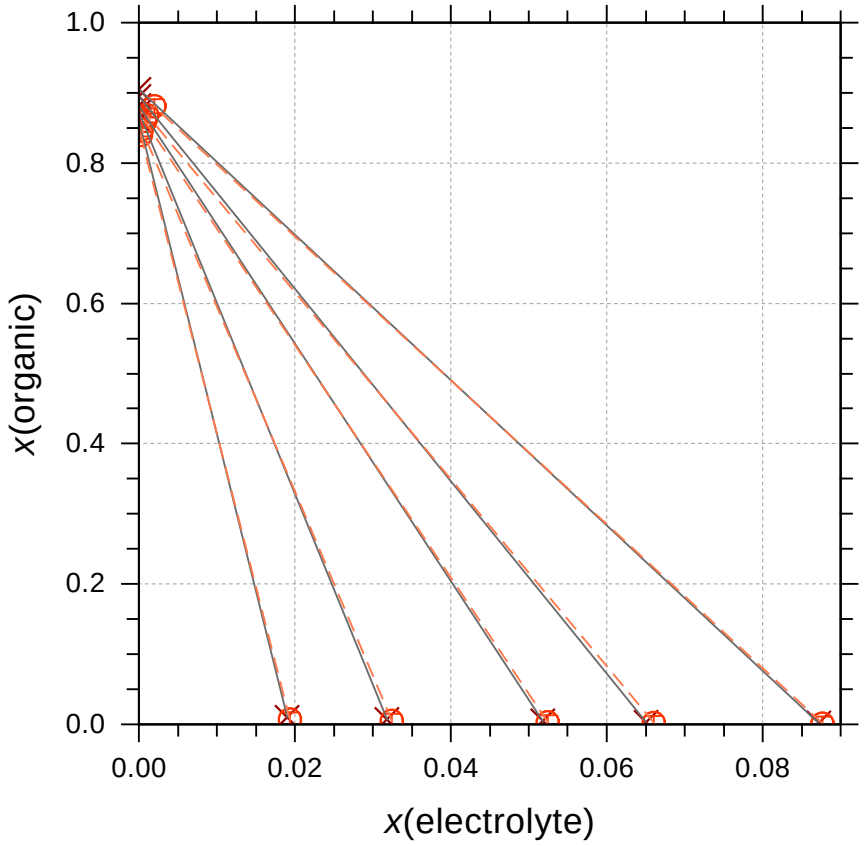
H_2O (1) + Ethyl_acetate (2) + NaCl (3)

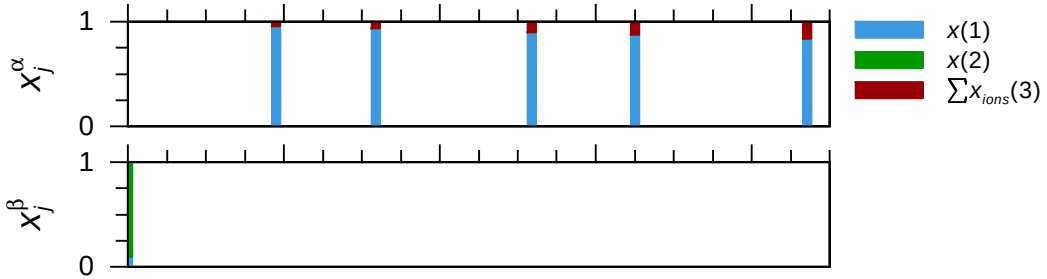
Temperature: 303 K

left y-axis:

× NaCl+EthylAcetate+Water_LLE_Gomis

○ AIOMFAC calc. LLE composition





initial weighting of dataset:

w^{init}(0348) = 1.000

dataset contribution to F_{obj}:

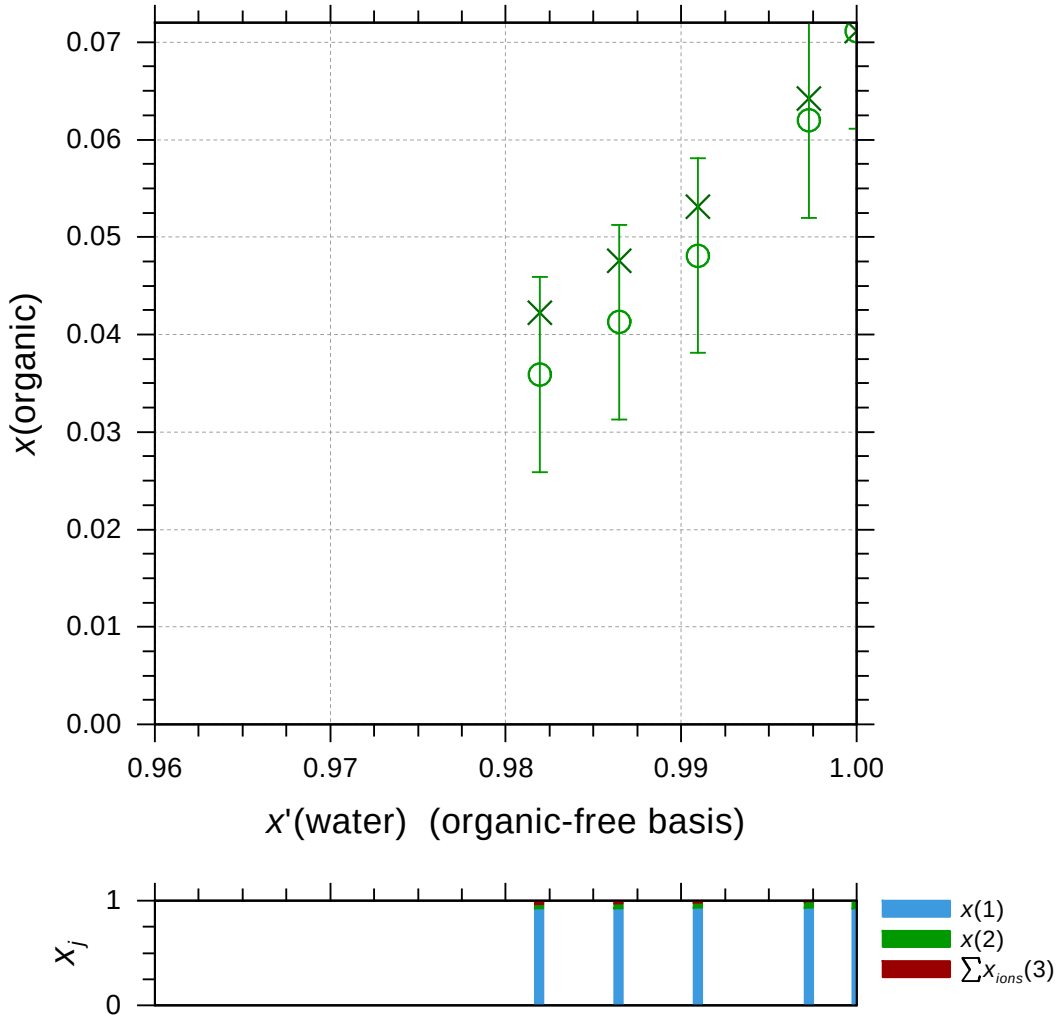
fval(0348) = 7.2358E+00

rel. contribution = 3.4409 %

Fig. S0391 (AIOMFAC_output_0416)

H_2O (1) + Methyl_acetate (2) + NaCl (3)

Temperature: 298 K

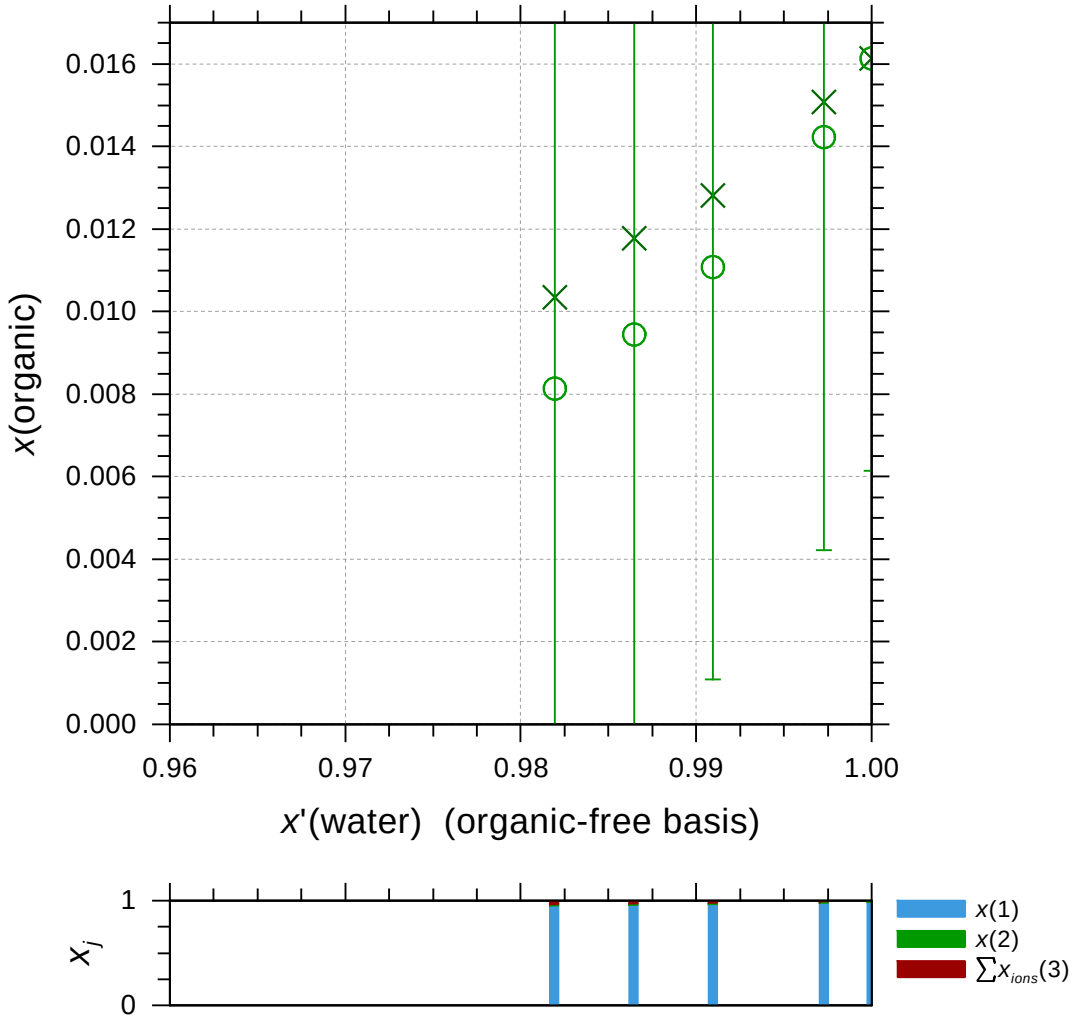


initial weighting of dataset:
w^{init}(0416) = 1.000
dataset contribution to F_{obj}:
fval(0416) = 3.4217E-02
rel. contribution = 0.0163 %

Fig. S0392 (AIOMFAC_output_0417)

H_2O (1) + Ethyl_acetate (2) + NaCl (3)

Temperature: 298 K

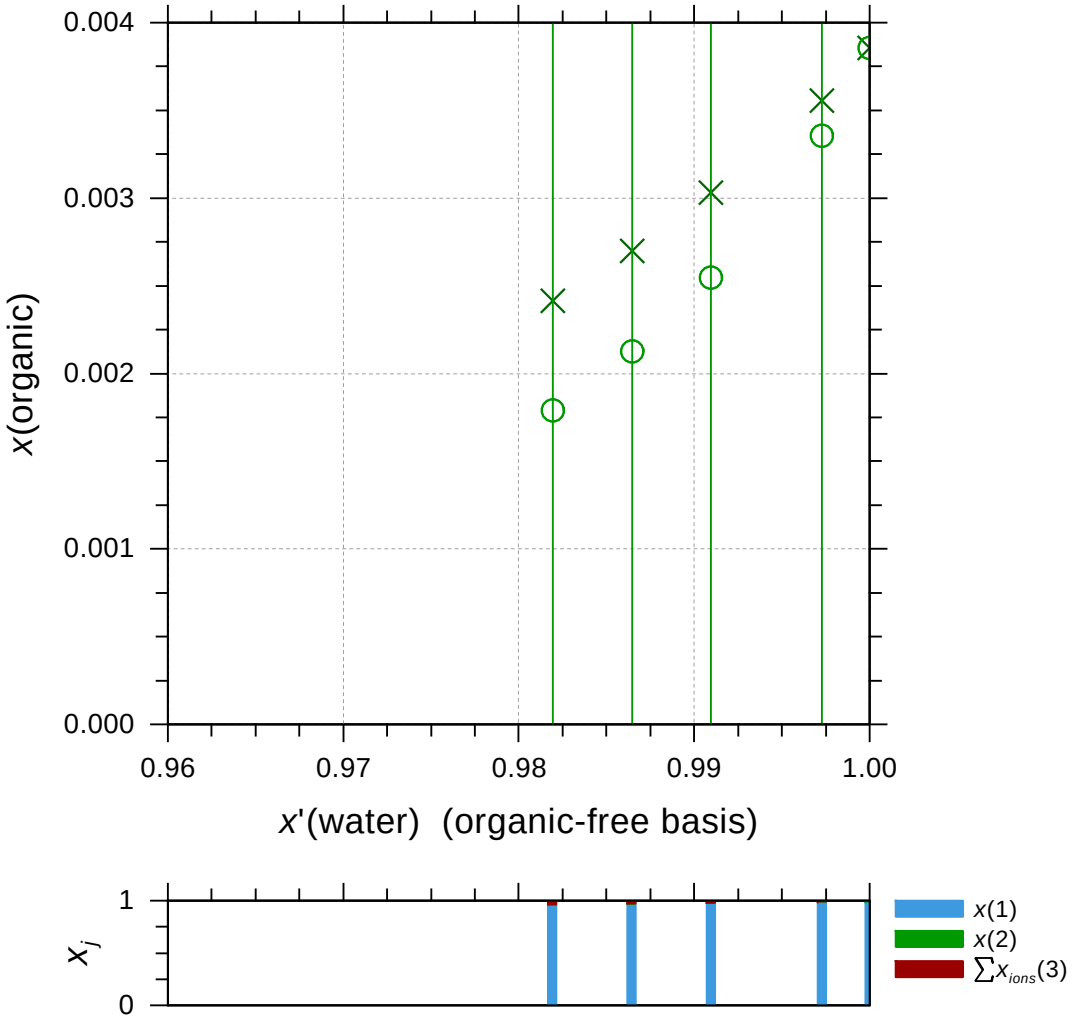


initial weighting of dataset:
$w^{init}(0417)$ = 1.000
dataset contribution to F_{obj}:
fval(0417) = 3.0031E-02
rel. contribution = 0.0143 %

Fig. S0393 (AIOMFAC_output_0418)

H_2O (1) + 1-Propyl_acetate (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0418)$ = 1.000

dataset contribution to F_{obj}:

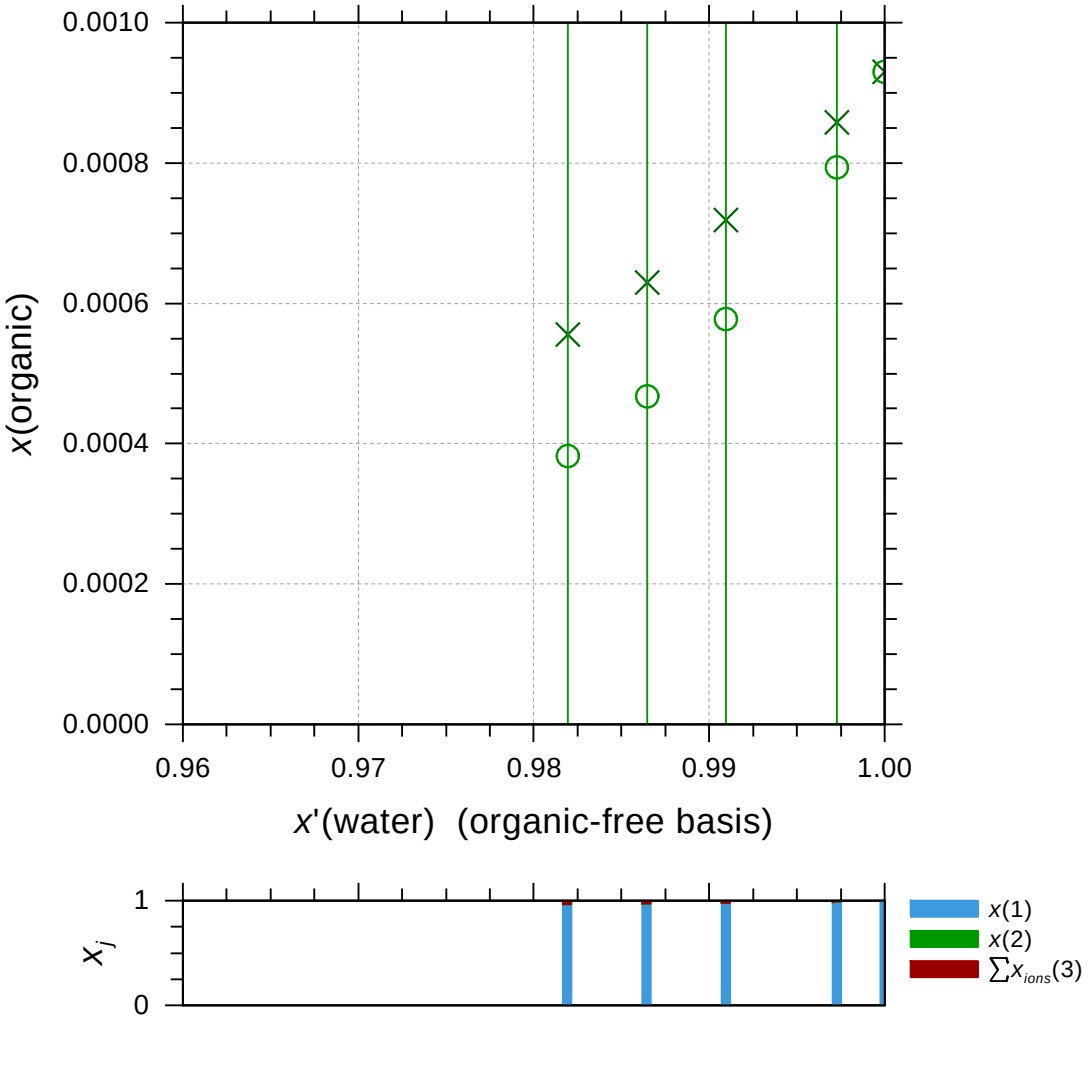
fval(0418) = 6.1856E-03

rel. contribution = 0.0029 %

Fig. S0394 (AIOMFAC_output_0419)

H_2O (1) + 1-Butyl_acetate (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0419)$ = 1.000

dataset contribution to F_{obj}:

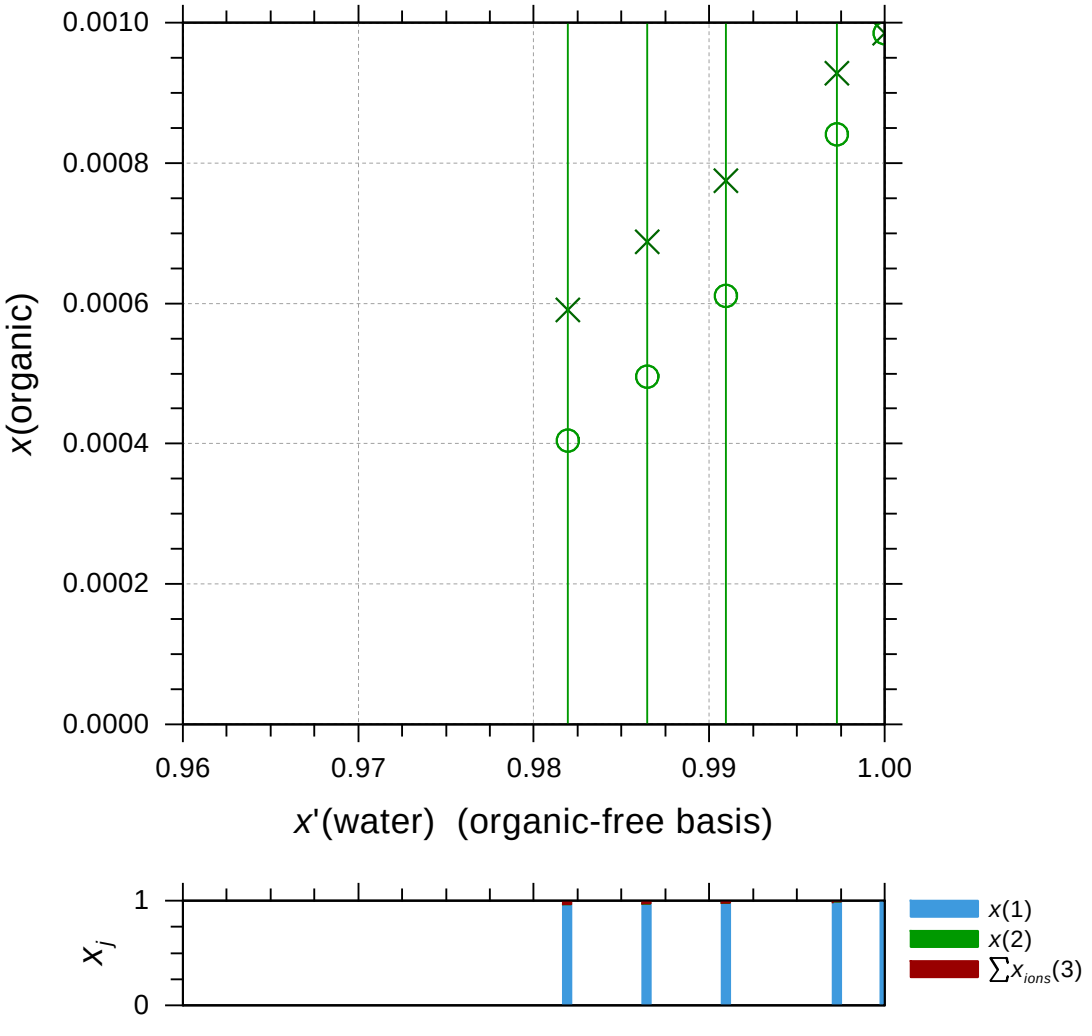
fval(0419) = 7.1286E-04

rel. contribution = 0.0003 %

Fig. S0395 (AIOMFAC_output_0420)

H_2O (1) + Isobutyl_acetate (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:

w^{init}(0420) = 1.000

dataset contribution to F_{obj}:

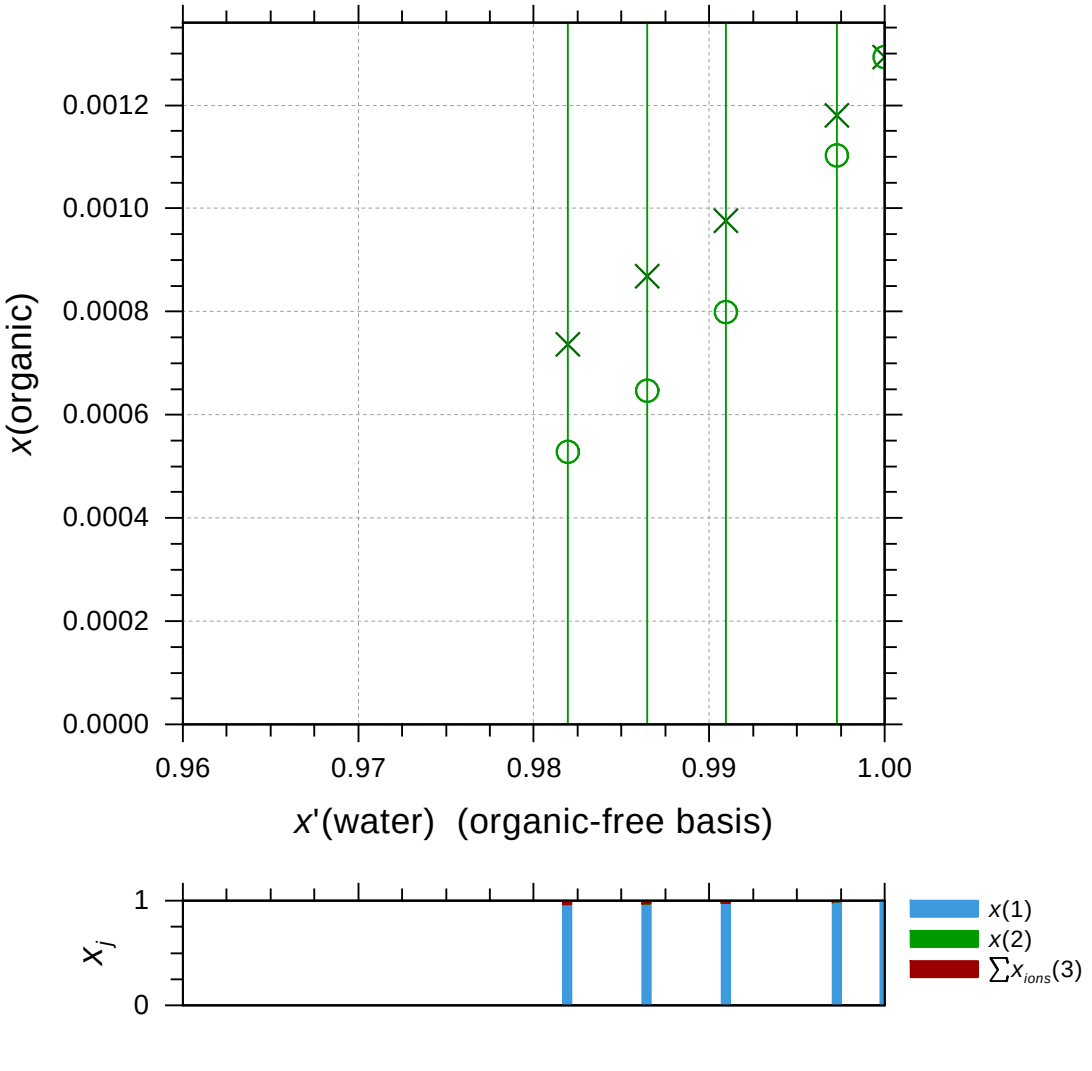
fval(0420) = 9.2637E-04

rel. contribution = 0.0004 %

Fig. S0396 (AIOMFAC_output_0421)

H_2O (1) + 2-Butyl_acetate (2) + NaCl (3)

Temperature: 298 K

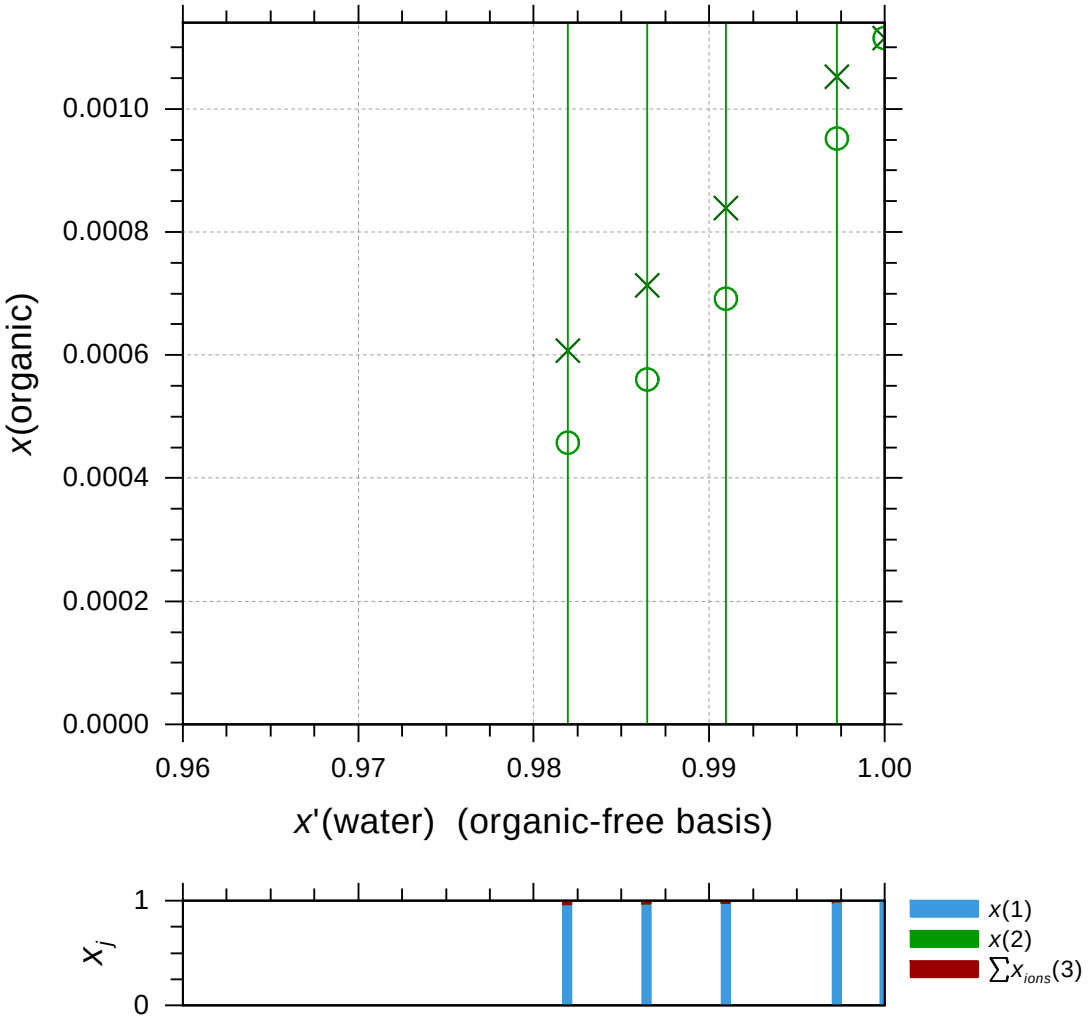


initial weighting of dataset:
$w^{init}(0421)$ = 1.000
dataset contribution to F_{obj}:
fval(0421) = 1.1019E-03
rel. contribution = 0.0005 %

Fig. S0397 (AIOMFAC_output_0422)

H_2O (1) + tert-Butyl_acetate (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:

w^{init}(0422) = 1.000

dataset contribution to F_{obj}:

fval(0422) = 6.6980E-04

rel. contribution = 0.0003 %

Fig. S0398 (AIOMFAC_output_0423)

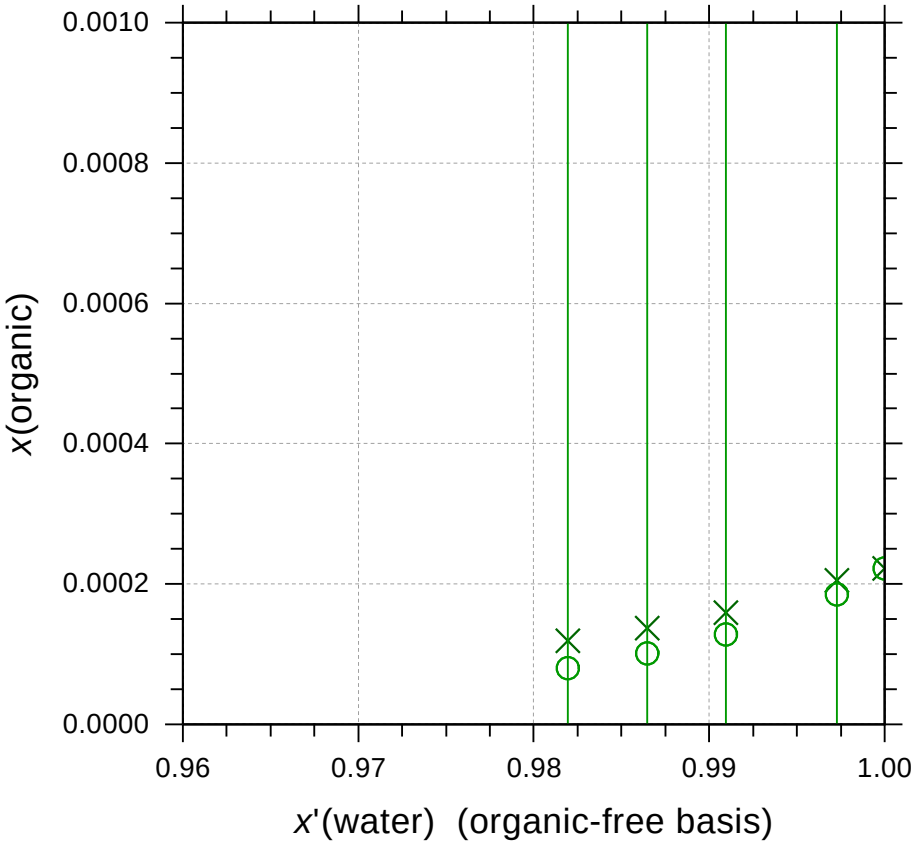
H_2O (1) + 1-Pentyl_acetate (2) + NaCl (3)

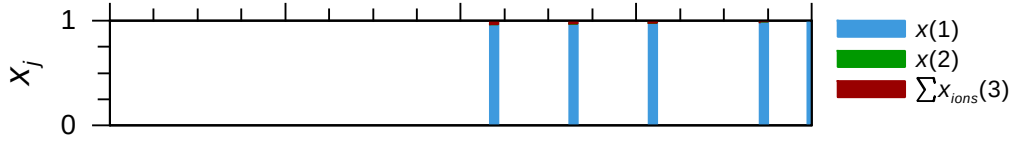
Temperature: 298 K

left y-axis:

× NaCl+1-PentylAcetate+Water_SLE_Segatin

○ AIOMFAC calc. SLE composition





initial weighting of dataset:

w^{init}(0423) = 1.000

dataset contribution to F_{obj}:

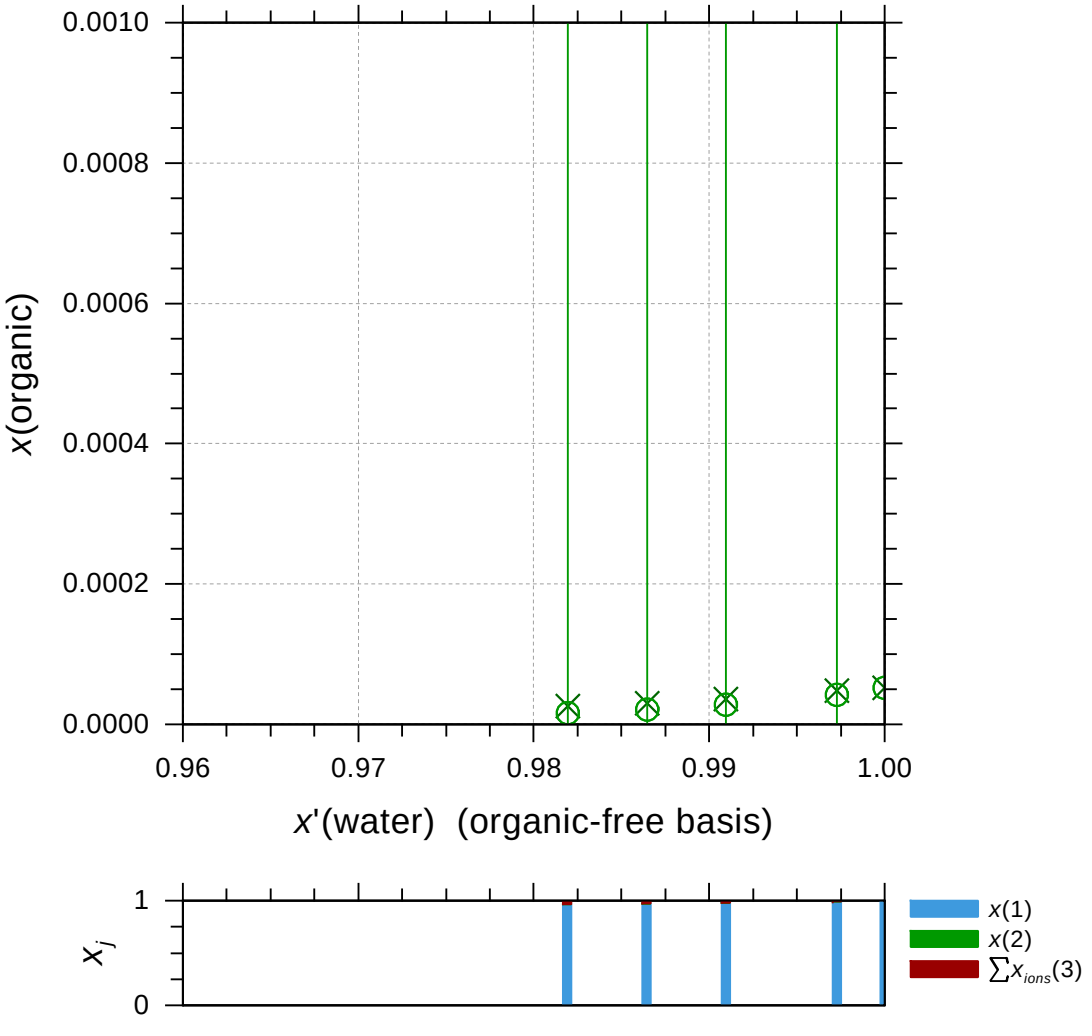
fval(0423) = 4.0963E-05

rel. contribution = 0.0000 %

Fig. S0399 (AIOMFAC_output_0424)

H_2O (1) + 1-Hexyl_acetate (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0424)$ = 1.000

dataset contribution to F_{obj}:

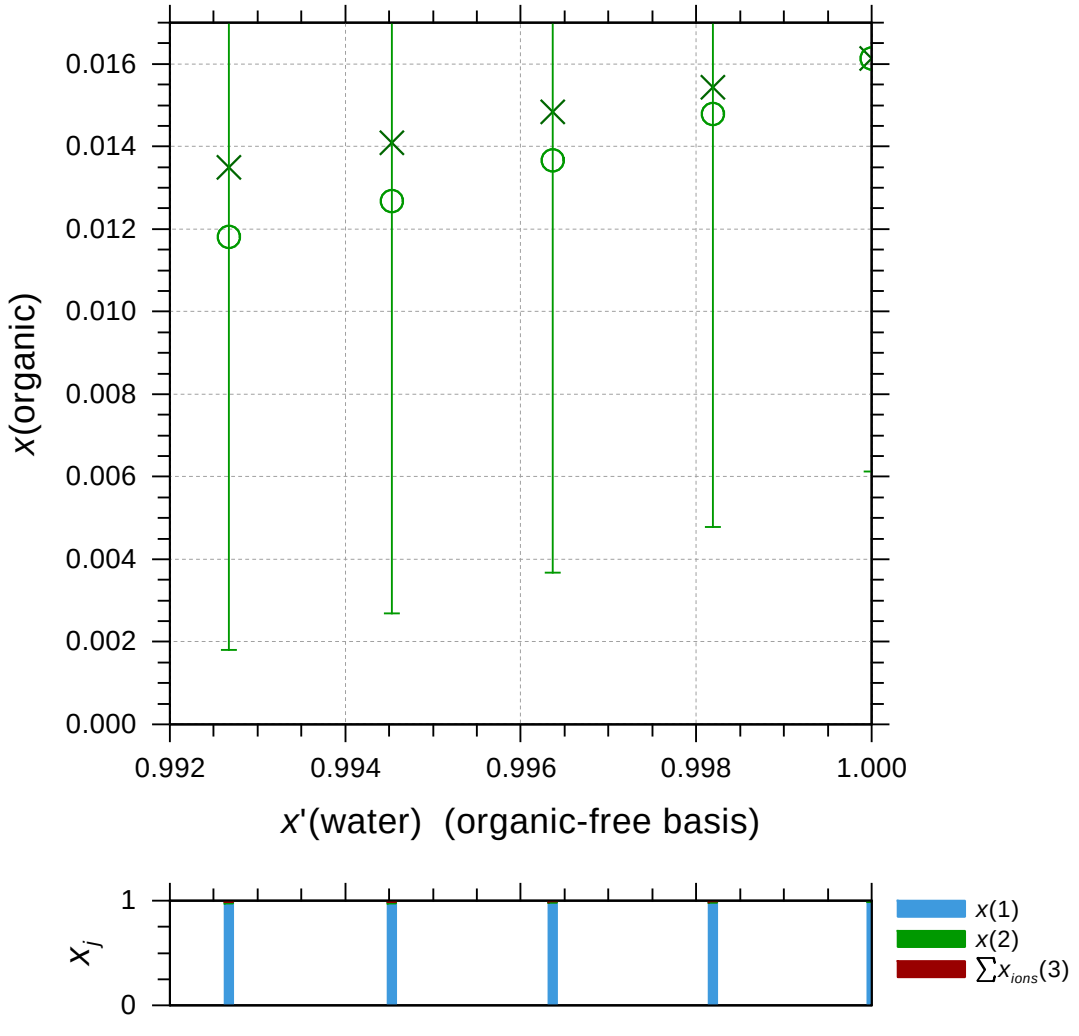
fval(0424) = 2.7568E-06

rel. contribution = 0.0000 %

Fig. S0400 (AIOMFAC_output_0430)

H_2O (1) + Ethyl_acetate (2) + NaCl (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0430)$ = 1.000

dataset contribution to F_{obj}:

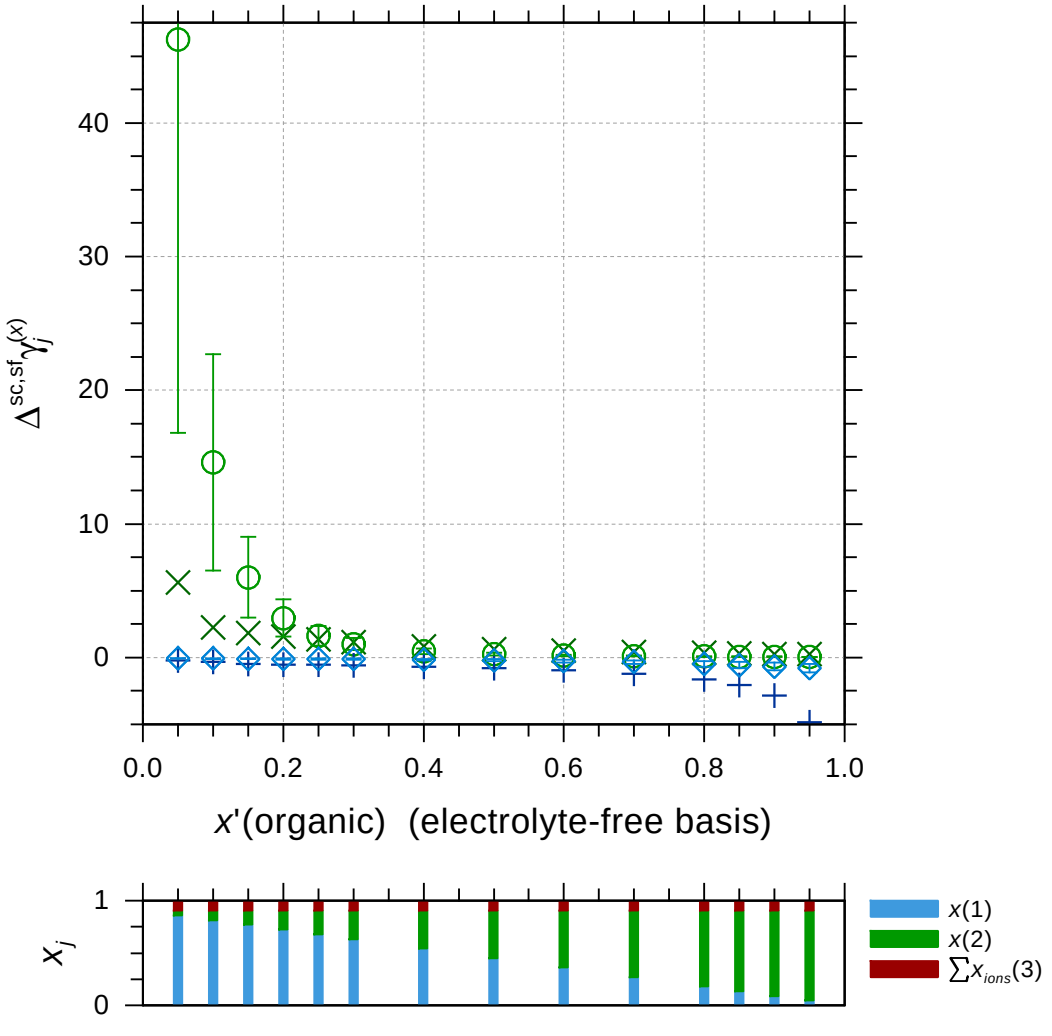
fval(0430) = 1.1387E-02

rel. contribution = 0.0054 %

Fig. S0401 (AIOMFAC_output_0914)

H_2O (1) + Ethyl_acetate (2) + NaCl (3)

Temperature range: 343 -- 347 K

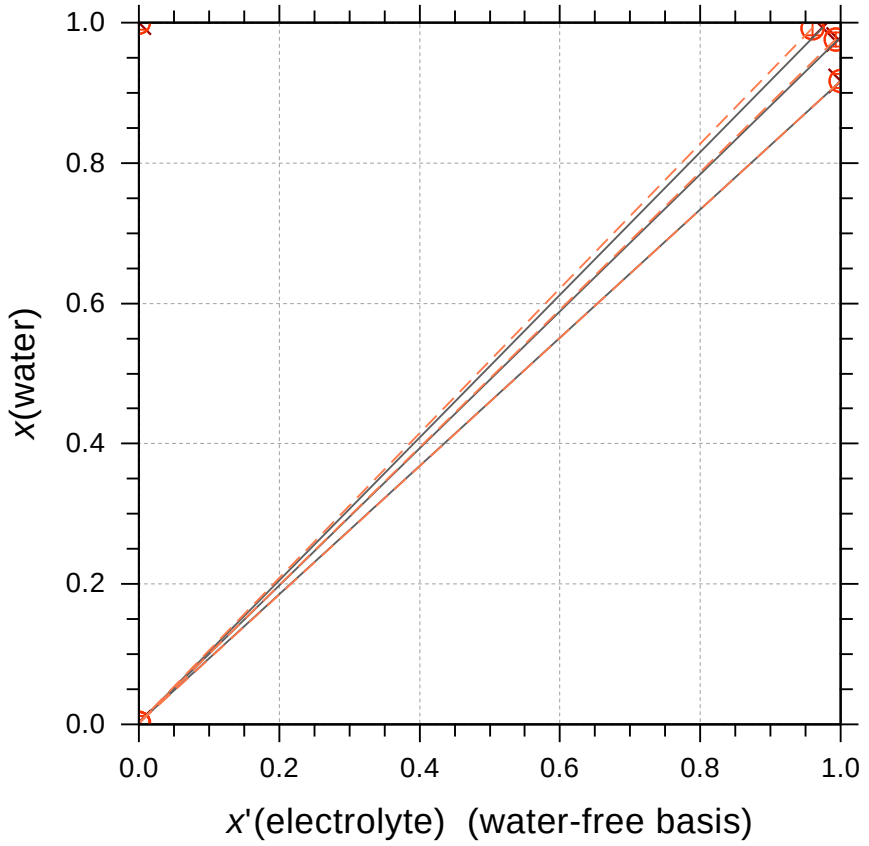


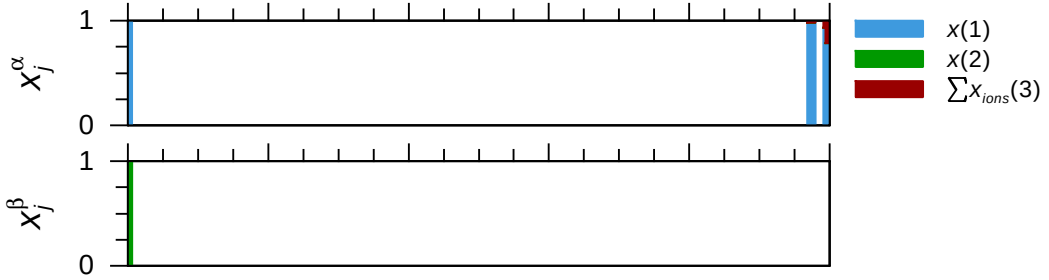
initial weighting of dataset:
w^{init}(0914) = 0.500
dataset contribution to F_{obj}:
fval(0914) = 1.8636E+00
rel. contribution = 0.8862 %

Fig. S0402 (AIOMFAC_output_0487)

H_2O (1) + Benzene (2) + $(NH_4)_2SO_4$ (3)

Temperature: 293 K





left y-axis:

× (NH4)2SO4+Benzene+Water_LLE_293K_vanDelden

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0487) = 1.000

dataset contribution to F_{obj}:

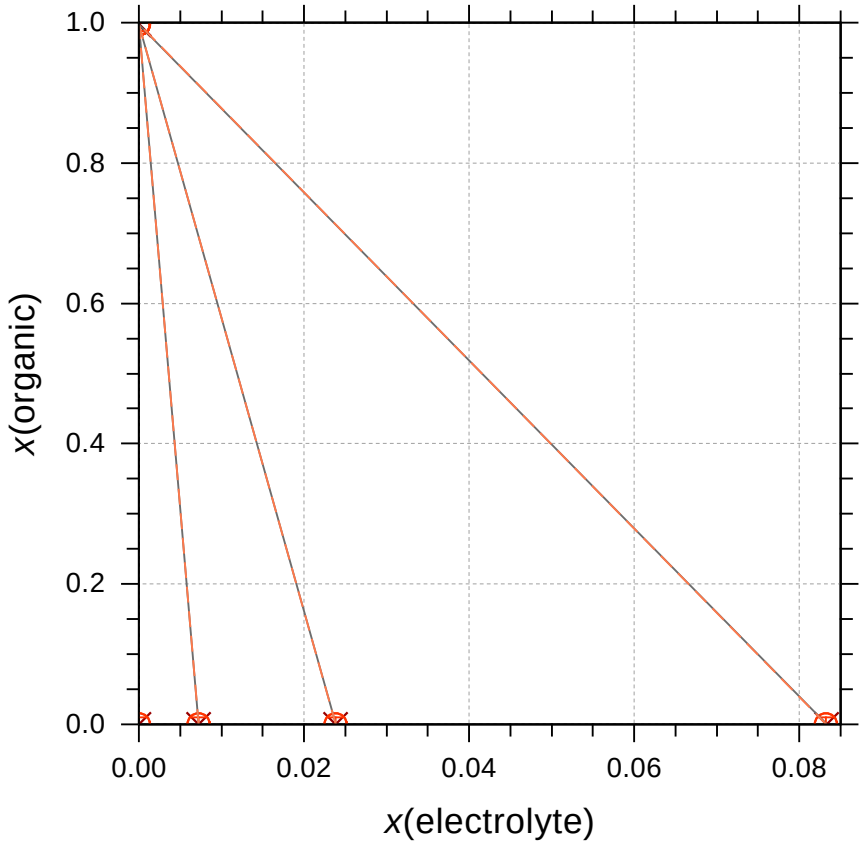
fval(0487) = 8.9224E-03

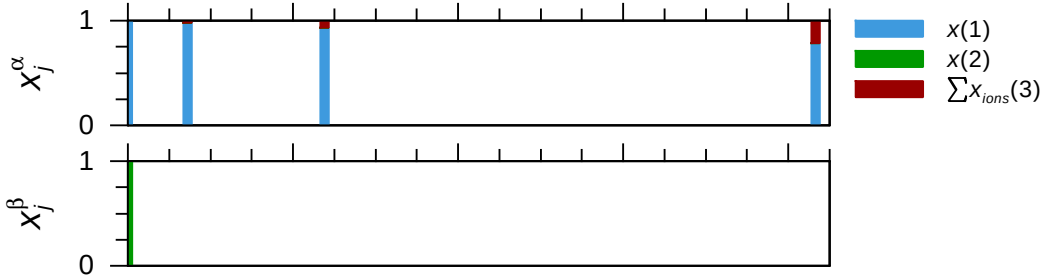
rel. contribution = 0.0042 %

Fig. S0402a (AIOMFAC_output_0487)

H_2O (1) + Benzene (2) + $(NH_4)_2SO_4$ (3)

Temperature: 293 K





left y-axis:

× (NH4)2SO4+Benzene+Water_LLE_293K_vanDelden

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0487) = 1.000

dataset contribution to F_{obj}:

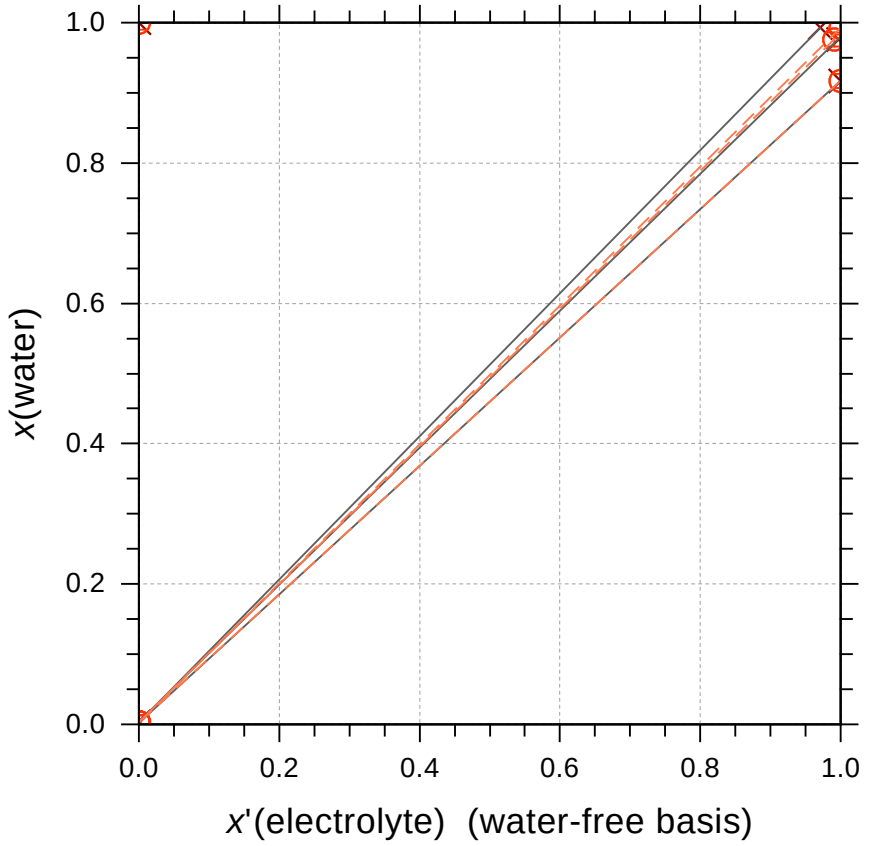
fval(0487) = 8.9224E-03

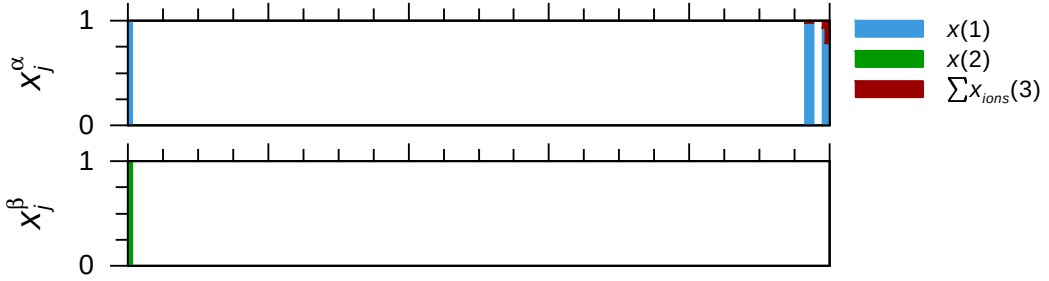
rel. contribution = 0.0042 %

Fig. S0403 (AIOMFAC_output_0488)

H_2O (1) + Benzene (2) + $(NH_4)_2SO_4$ (3)

Temperature: 313 K





left y-axis:

× (NH4)2SO4+Benzene+Water_LLE_313K_vanDelden

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0488) = 0.800

dataset contribution to F_{obj}:

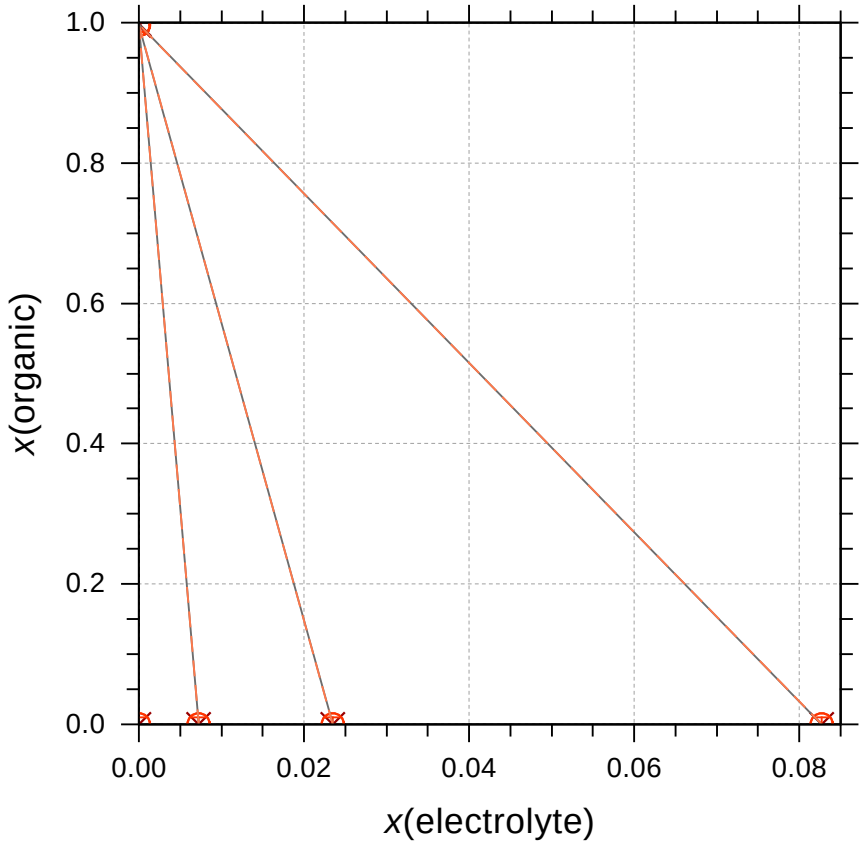
fval(0488) = 1.0157E-02

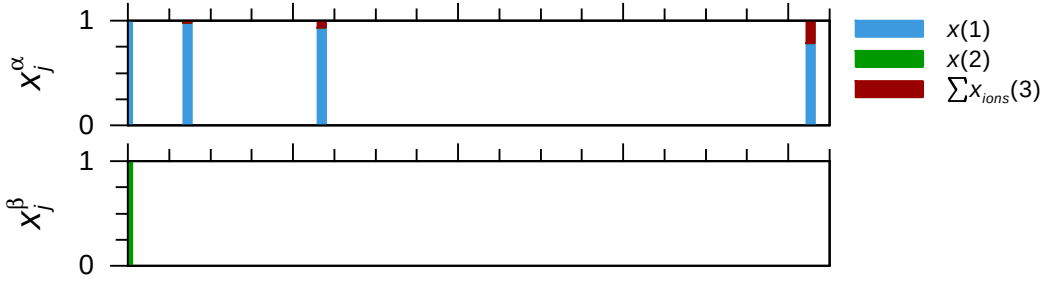
rel. contribution = 0.0048 %

Fig. S0403a (AIOMFAC_output_0488)

H_2O (1) + Benzene (2) + $(NH_4)_2SO_4$ (3)

Temperature: 313 K





left y-axis:

× (NH4)2SO4+Benzene+Water_LLE_313K_vanDelden

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0488) = 0.800

dataset contribution to F_{obj}:

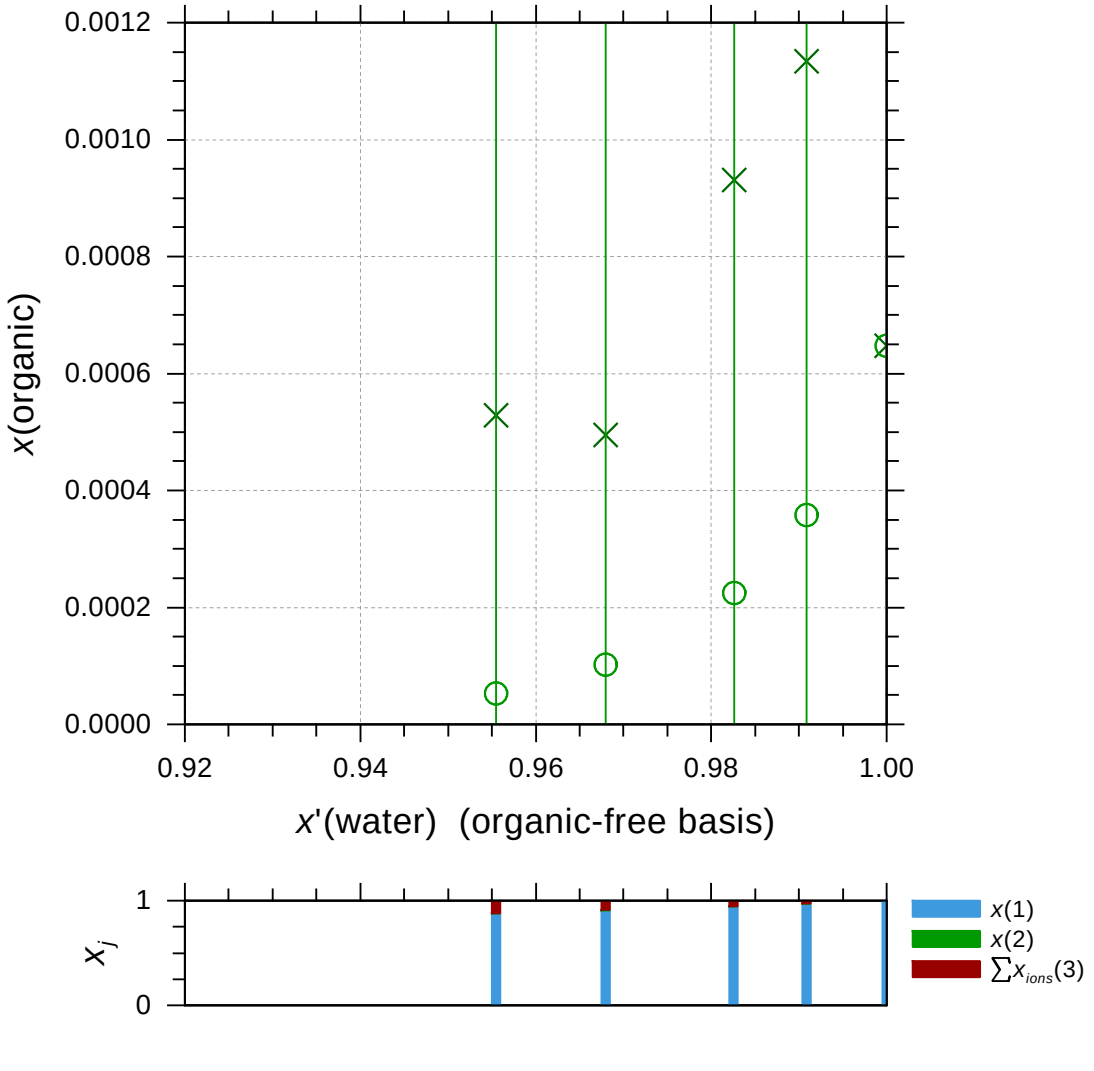
fval(0488) = 1.0157E-02

rel. contribution = 0.0048 %

Fig. S0404 (AIOMFAC_output_0978)

H_2O (1) + 2,4-Dihydroxybenzaldehyde (2) + $Ca(NO_3)_2$ (3)

Temperature: 298 K

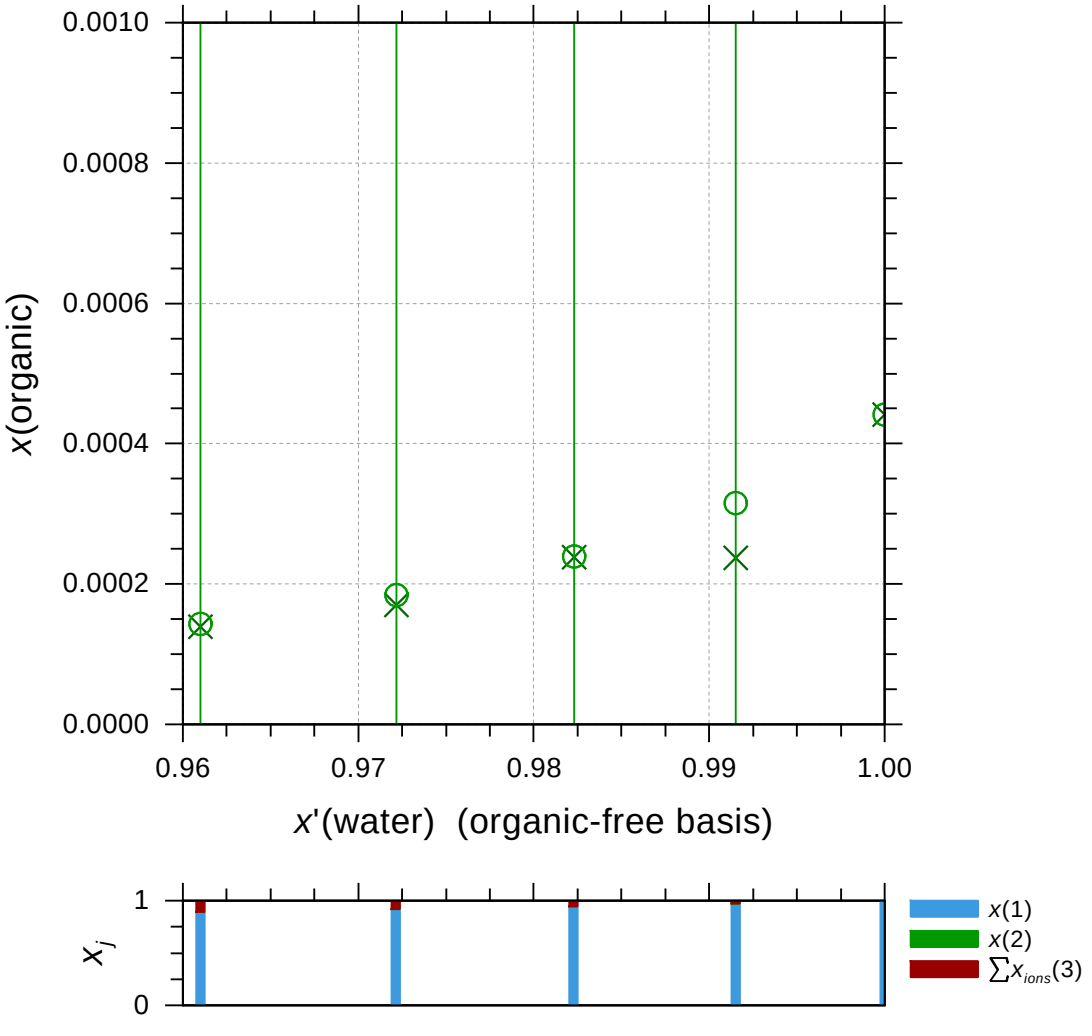


initial weighting of dataset:
$w^{init}(0978)$ = 1.000
dataset contribution to F_{obj}:
fval(0978) = 1.2474E-02
rel. contribution = 0.0059 %

Fig. S0405 (AIOMFAC_output_0924)

H_2O (1) + Benzene (2) + $CaCl_2$ (3)

Temperature: 303 K

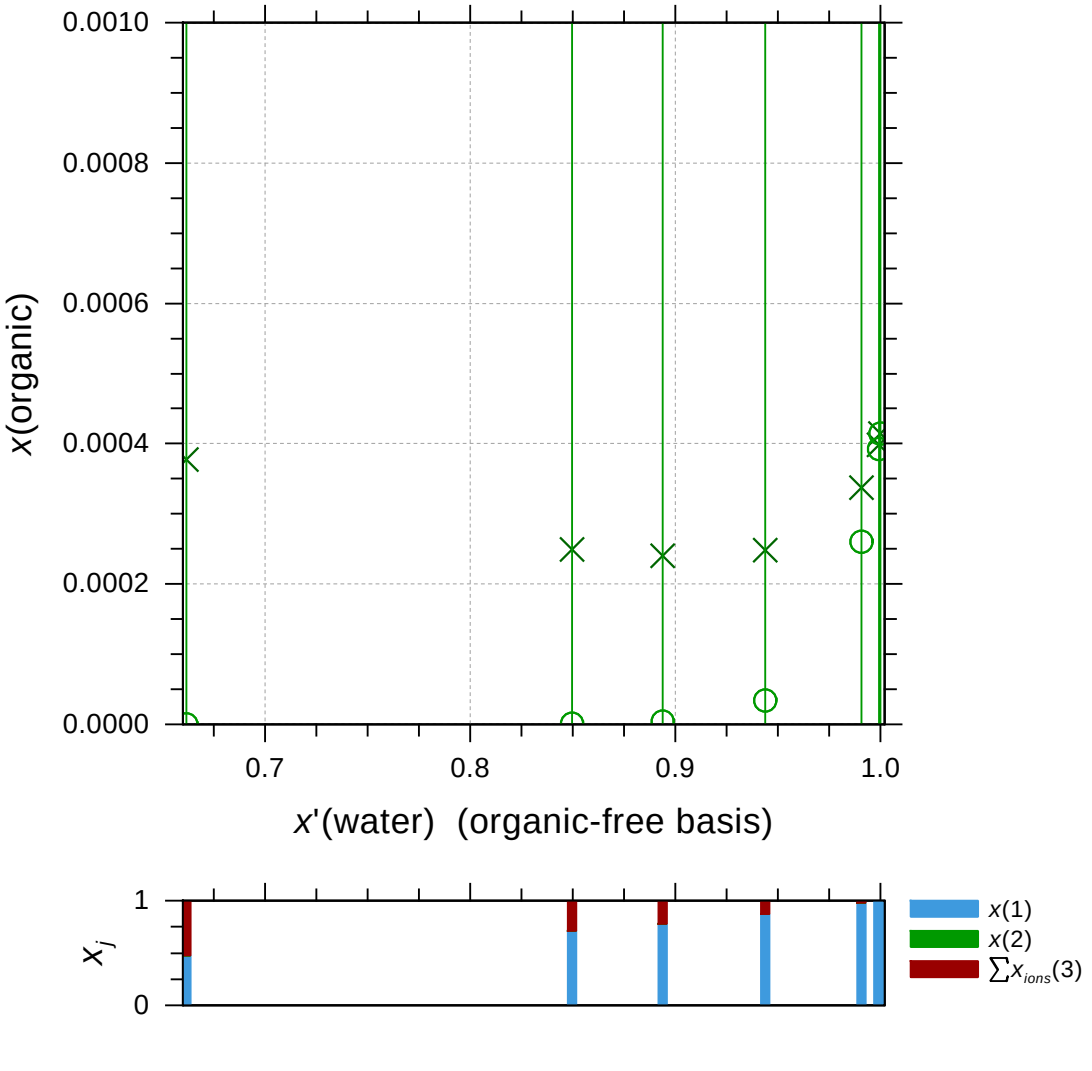


initial weighting of dataset:
$w^{init}(0924)$ = 0.800
dataset contribution to F_{obj}:
fval(0924) = 4.8375E-05
rel. contribution = 0.0000 %

Fig. S0406 (AIOMFAC_output_0490)

H_2O (1) + Benzene (2) + H_2SO_4 (3)

Temperature: 303 K

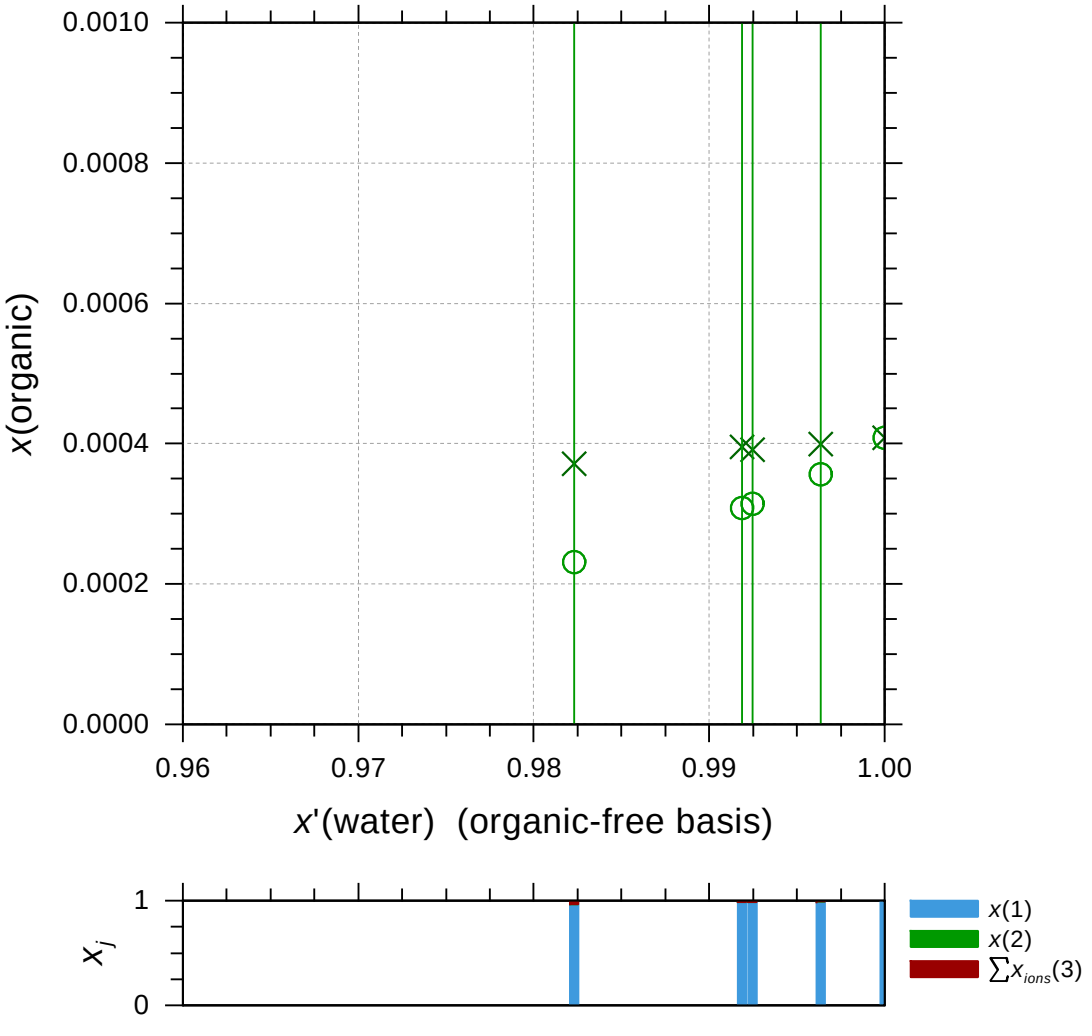


initial weighting of dataset:
$w^{init}(0490)$ = 0.200
dataset contribution to F_{obj}:
fval(0490) = 5.8636E-04
rel. contribution = 0.0003 %

Fig. S0407 (AIOMFAC_output_0471)

H_2O (1) + Benzene (2) + HCl (3)

Temperature: 298 K

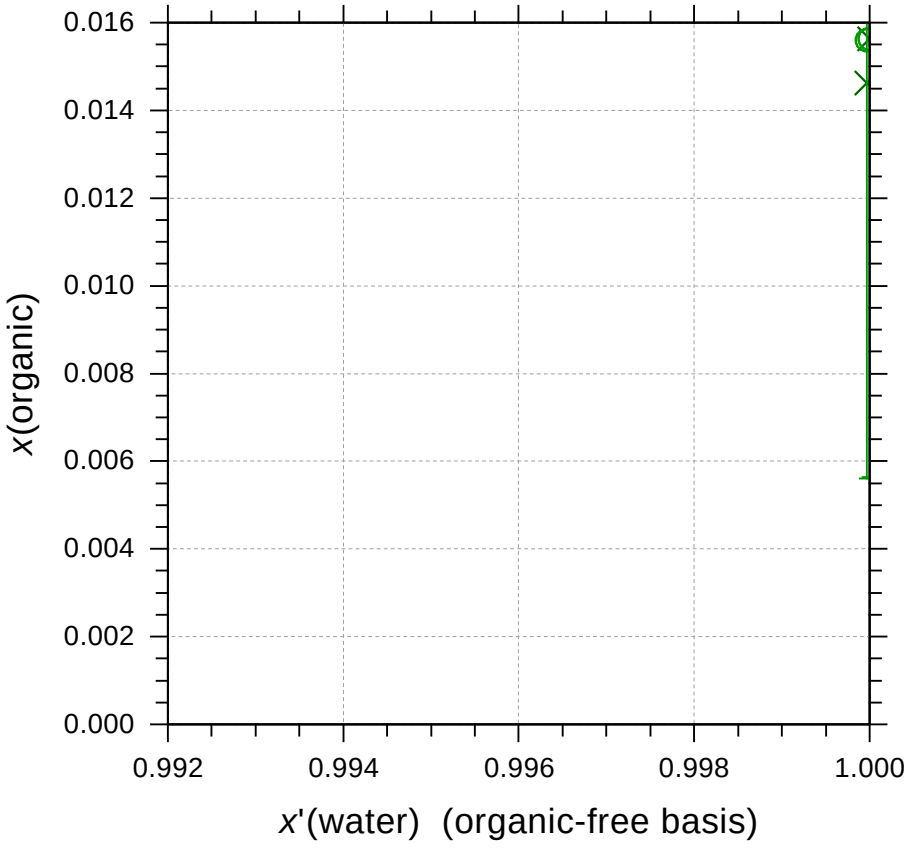


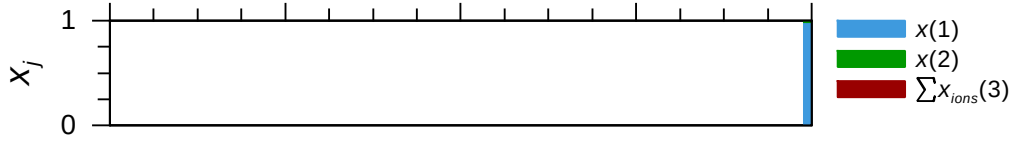
initial weighting of dataset:
$w^{init}(0471)$ = 1.000
dataset contribution to F_{obj}:
fval(0471) = 3.2615E-04
rel. contribution = 0.0002 %

Fig. S0408 (AIOMFAC_output_0484)

H_2O (1) + Phenol (2) + HCl (3)

Temperature: 300 K





left y-axis:

× HCl+Phenol+Water_Solubility_Jaoui

○ AIOMFAC calc. SLE composition

initial weighting of dataset:

w^{init}(0484) = 1.000

dataset contribution to F_{obj}:

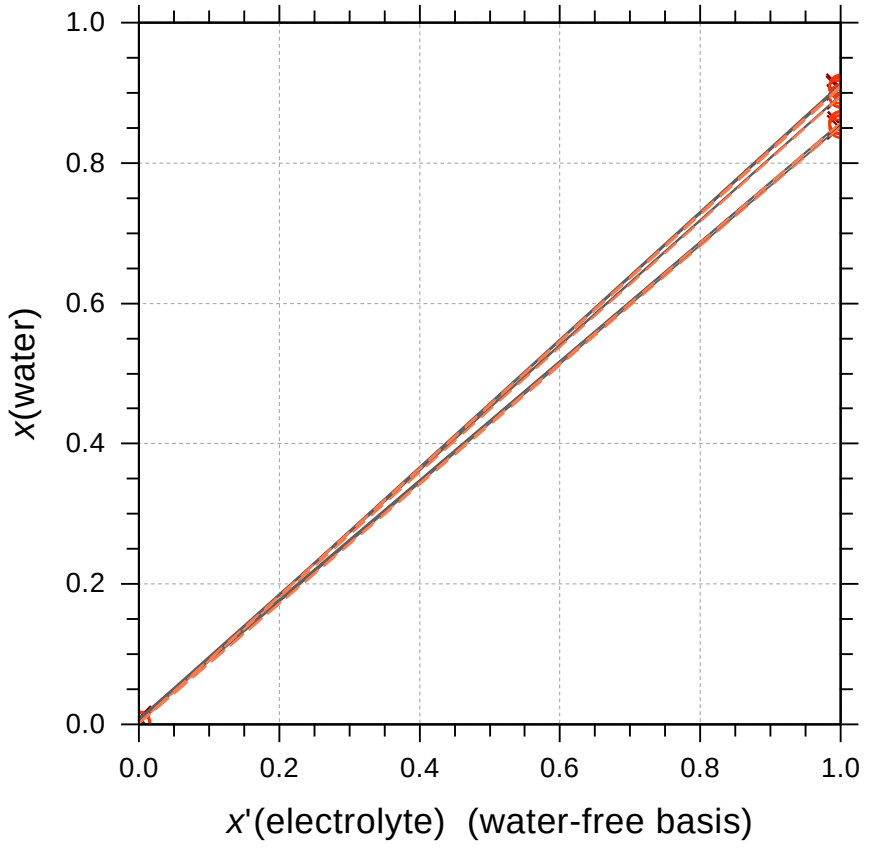
fval(0484) = 1.6194E-03

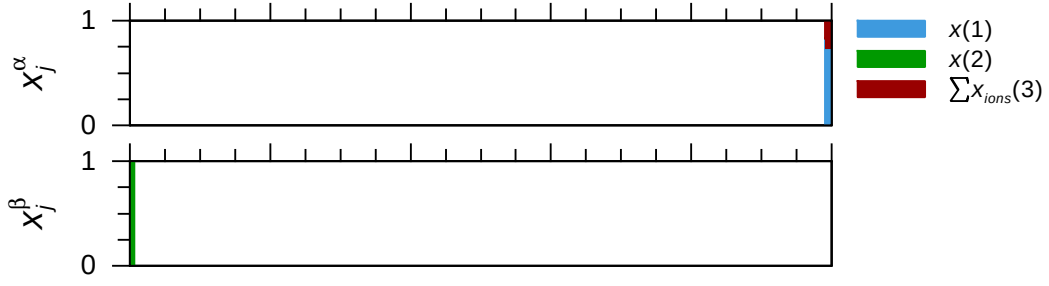
rel. contribution = 0.0008 %

Fig. S0409 (AIOMFAC_output_0485)

H_2O (1) + Benzene (2) + HCl (3)

Temperature: 303 K





left y-axis:

× HCl+Benzene+Water_LLE_Ishidao

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0485) = 0.000

dataset contribution to F_{obj}:

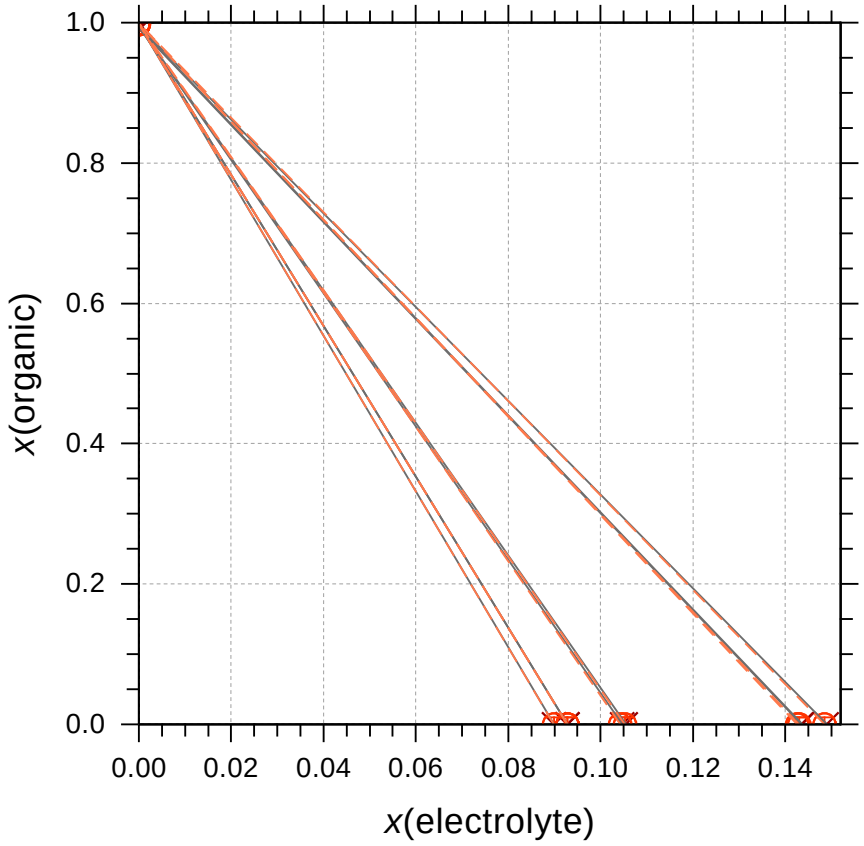
fval(0485) = 0.0000E+00

rel. contribution = 0.0000 %

Fig. S0409a (AIOMFAC_output_0485)

H_2O (1) + Benzene (2) + HCl (3)

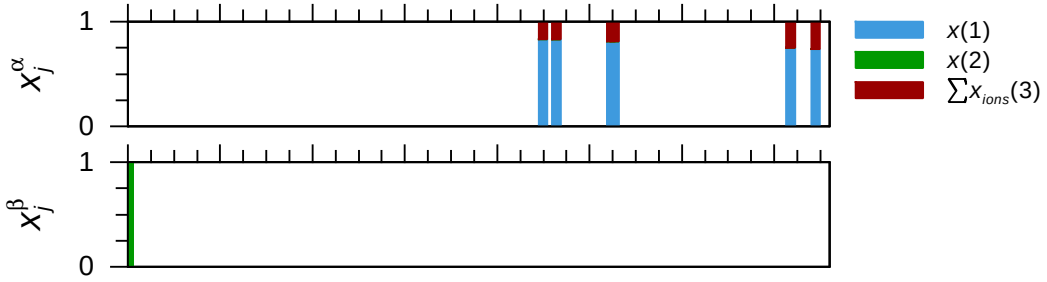
Temperature: 303 K



left y-axis:

× HCl+Benzene+Water_LLE_Ishidao

○ AIOMFAC calc. LLE composition



initial weighting of dataset:

w^{init}(0485) = 0.000

dataset contribution to F_{obj}:

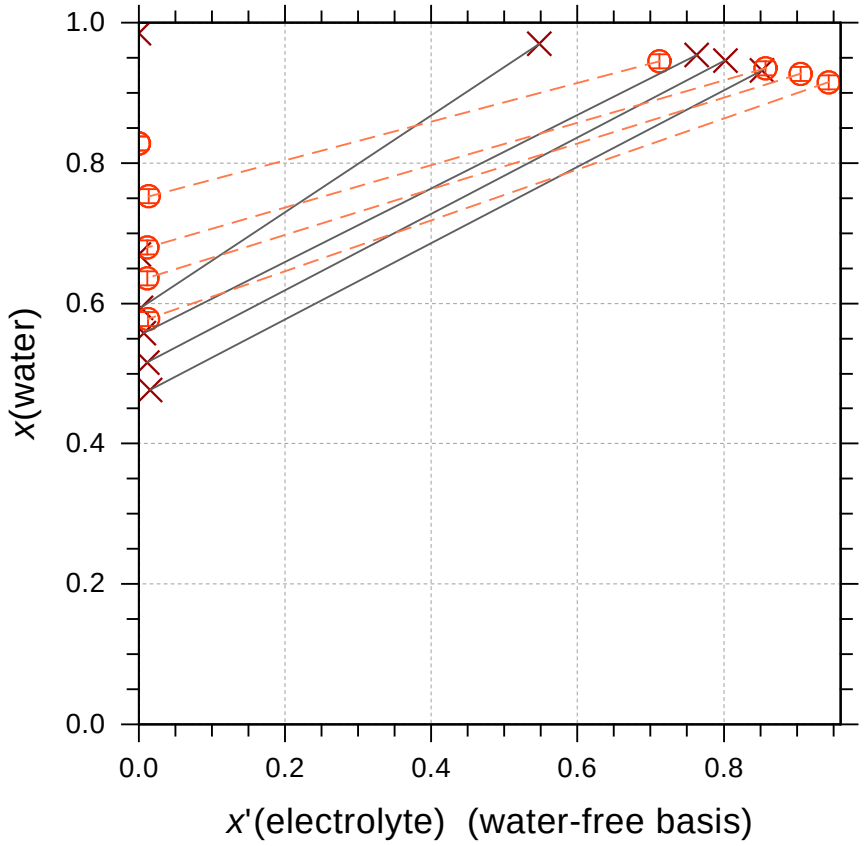
fval(0485) = 0.0000E+00

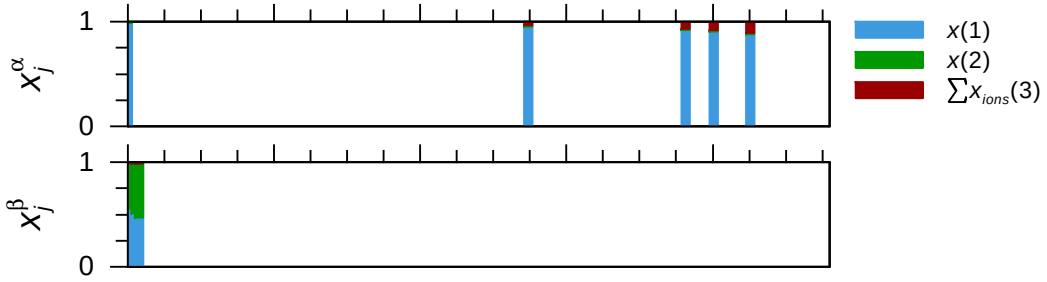
rel. contribution = 0.0000 %

Fig. S0410 (AIOMFAC_output_0486)

H_2O (1) + Phenol (2) + HCl (3)

Temperature: 285 K





left y-axis:

× HCl+Phenol+Water_LLE_Schreinemakers

○ AIOMFAC calc. LLE composition

initial weighting of dataset:

w^{init}(0486) = 0.800

dataset contribution to F_{obj}:

fval(0486) = 1.2208E+00

rel. contribution = 0.5805 %

Fig. S0410a (AIOMFAC_output_0486)

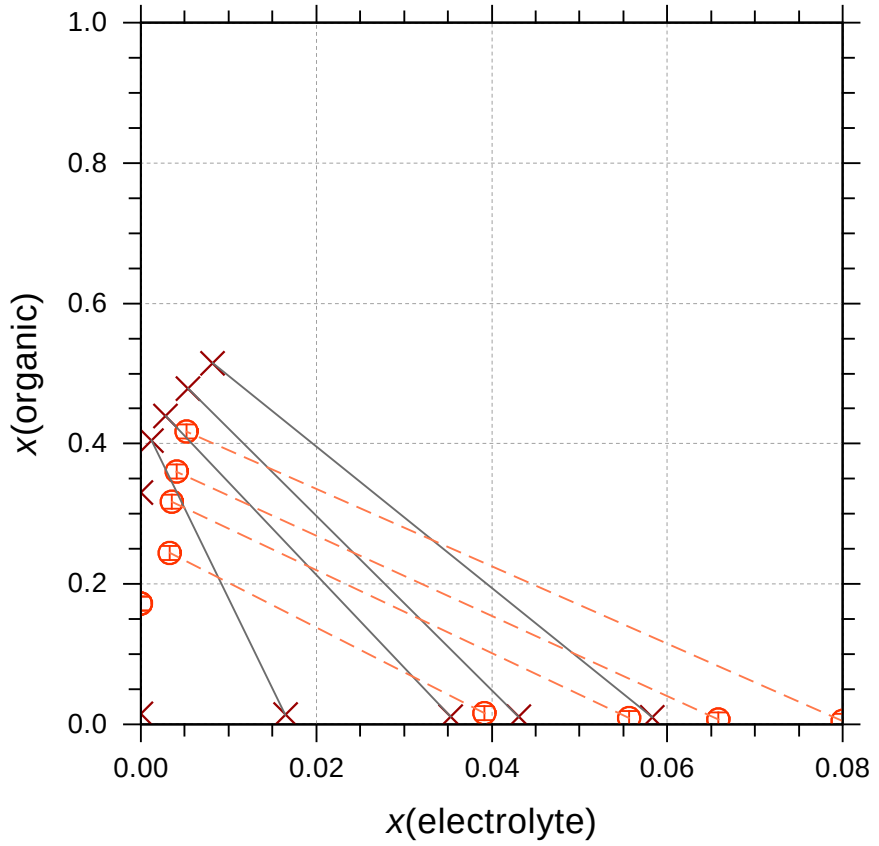
H_2O (1) + Phenol (2) + HCl (3)

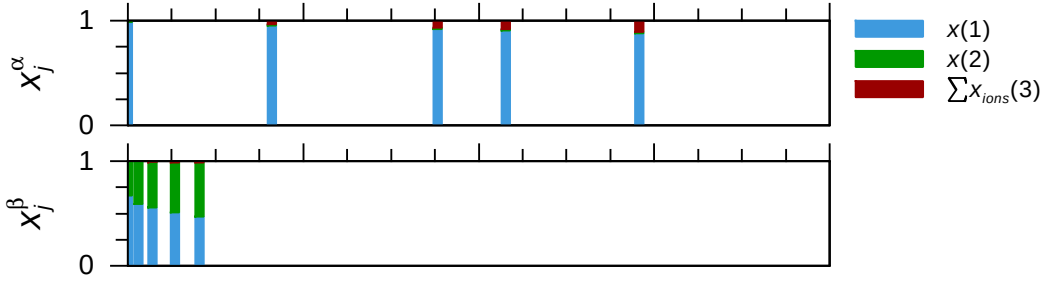
Temperature: 285 K

left y-axis:

× HCl+Phenol+Water_LLE_Schreinemakers

○ AIOMFAC calc. LLE composition



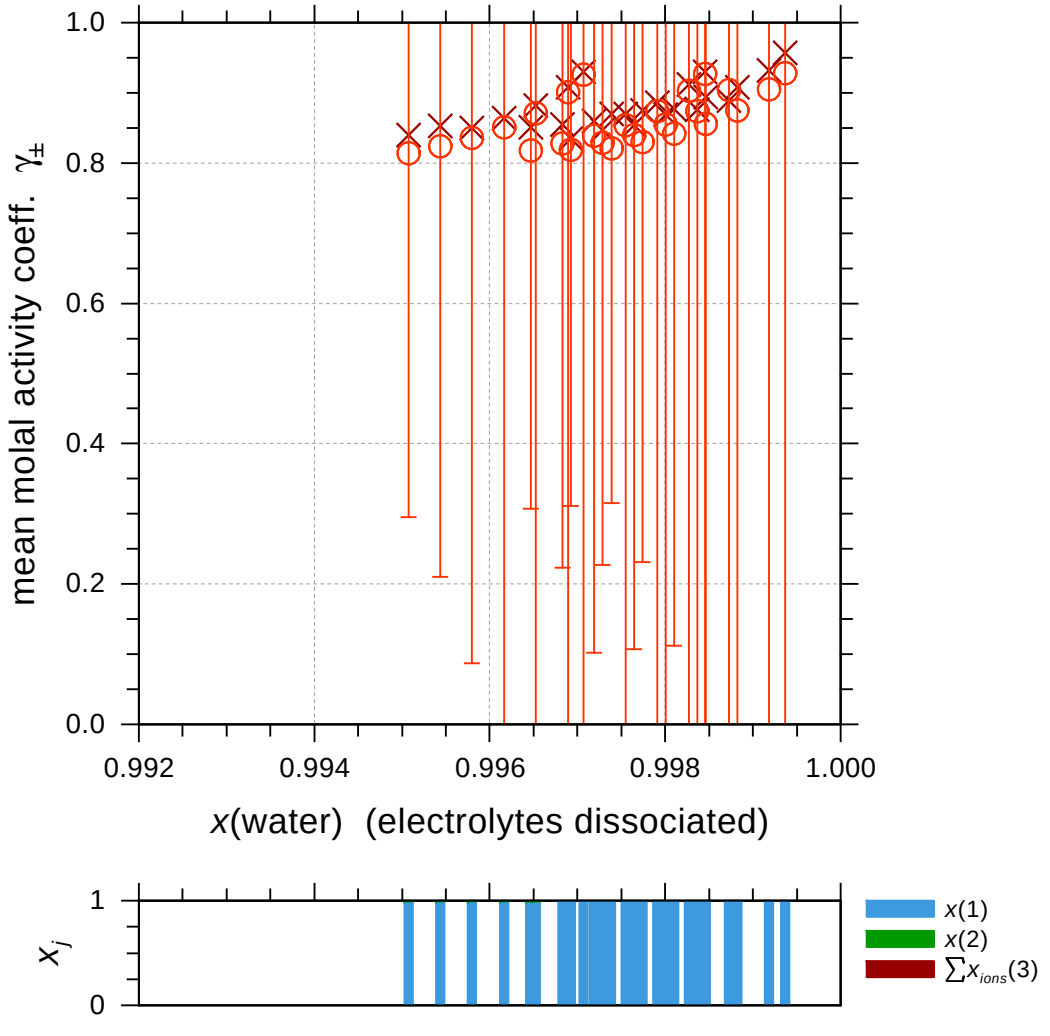


initial weighting of dataset:
w^{init}(0486) = 0.800
dataset contribution to F_{obj}:
fval(0486) = 1.2208E+00
rel. contribution = 0.5805 %

Fig. S0411 (AIOMFAC_output_1030)

H_2O (1) + Phenol (2) + HCl (3)

Temperature: 298 K

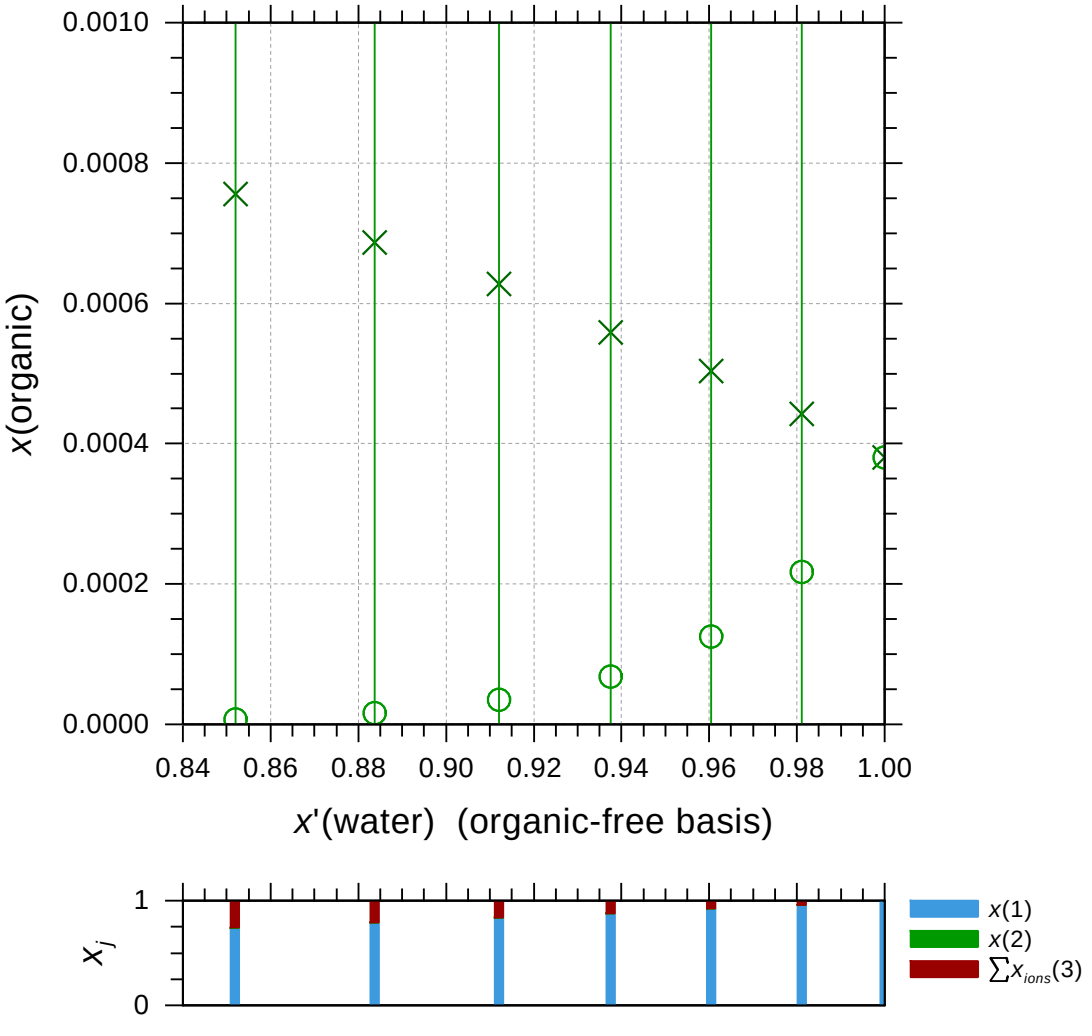


initial weighting of dataset:
$w^{init}(1030)$ = 2.000
dataset contribution to F_{obj}:
fval(1030) = 4.5069E-03
rel. contribution = 0.0021 %

Fig. S0412 (AIOMFAC_output_0489)

H_2O (1) + Benzene (2) + HNO_3 (3)

Temperature: 295 K

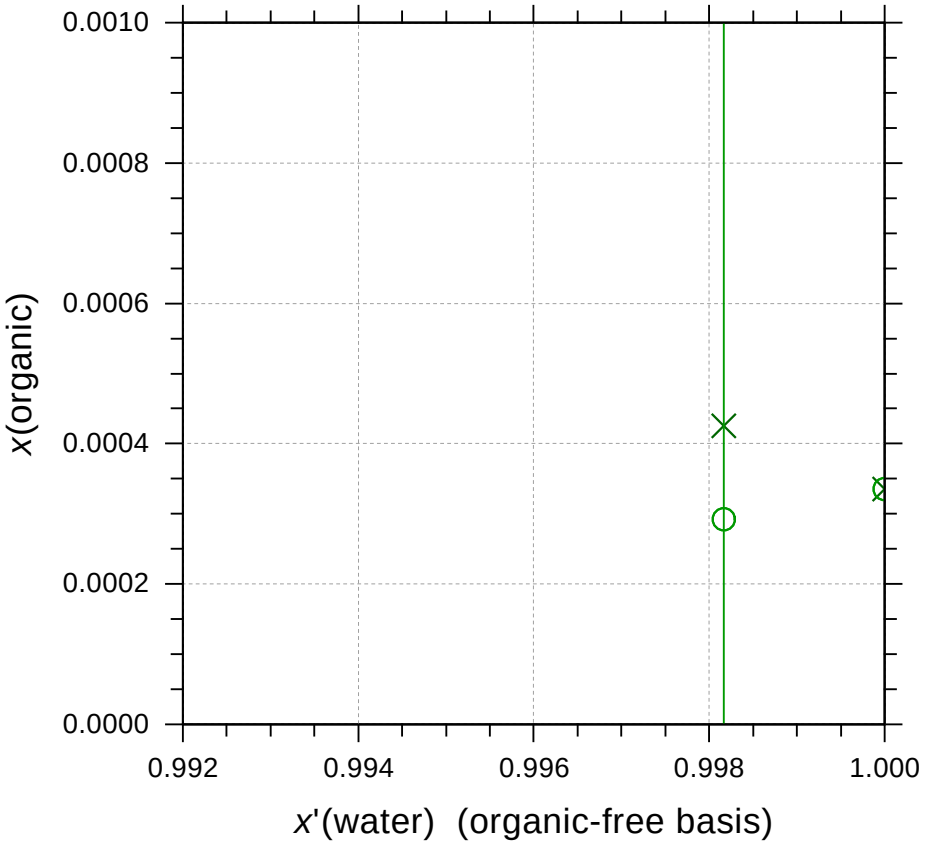


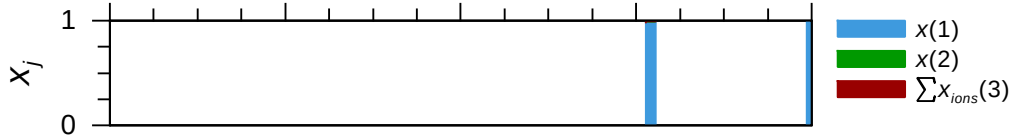
initial weighting of dataset:
$w^{init}(0489)$ = 0.500
dataset contribution to F_{obj}:
fval(0489) = 7.9080E-03
rel. contribution = 0.0038 %

Fig. S0413 (AIOMFAC_output_0494)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + K_2SO_4 (3)

Temperature: 298 K





left y-axis:

× K2SO4+2-HydroxybenzoicAcid+Water_SLE_Sugunan

○ AIOMFAC calc. SLE composition

initial weighting of dataset:

w^{init}(0494) = 1.000

dataset contribution to F_{obj}:

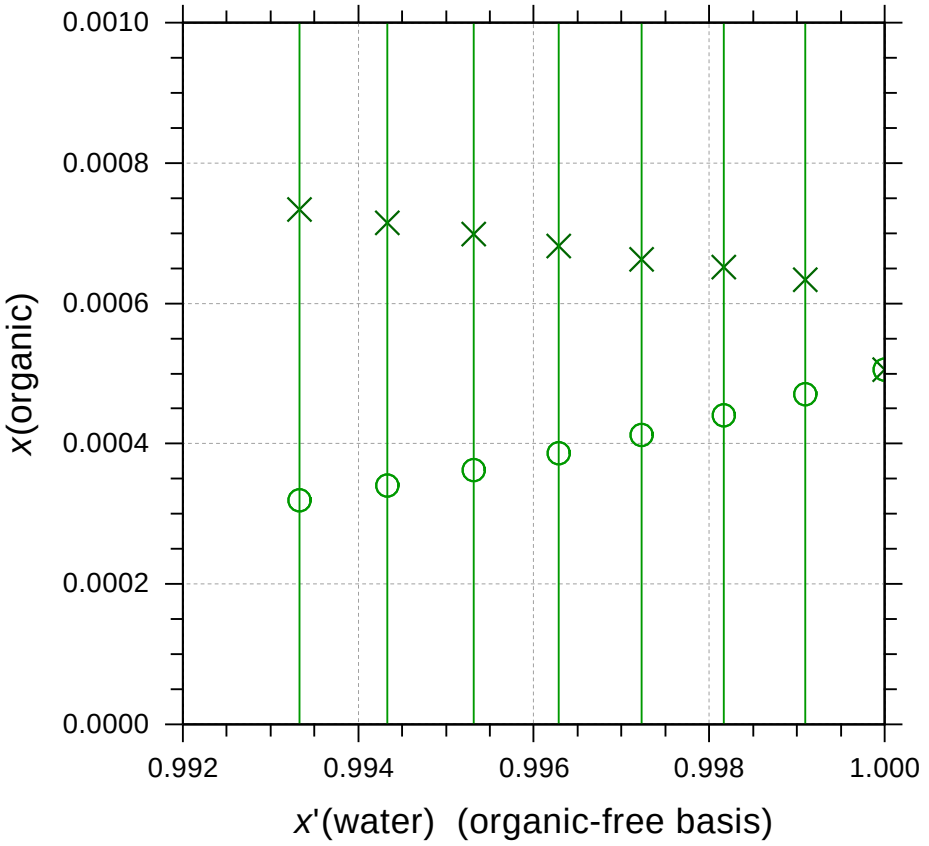
fval(0494) = 1.6504E-04

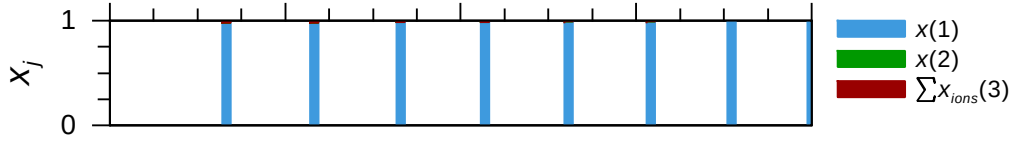
rel. contribution = 0.0001 %

Fig. S0414 (AIOMFAC_output_0499)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + K_2SO_4 (3)

Temperature: 308 K





left y-axis:

× K2SO4+2-HydroxybenzoicAcid+Water_SLE_308K_Sugunan

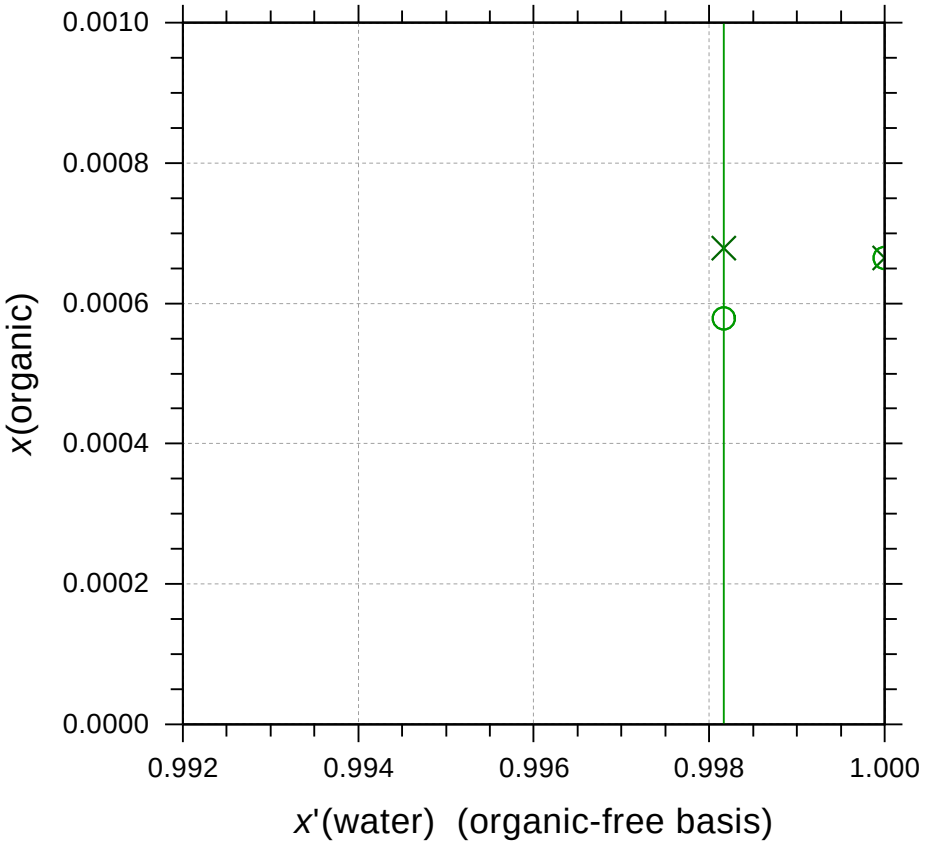
○ AIOMFAC calc. SLE composition

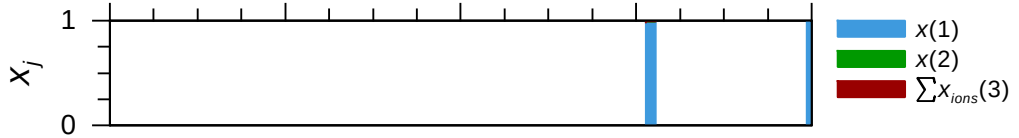
initial weighting of dataset:
w^{init}(0499) = 0.500
dataset contribution to F_{obj}:
fval(0499) = 2.8249E-03
rel. contribution = 0.0013 %

Fig. S0415 (AIOMFAC_output_0904)

H_2O (1) + 4-Hydroxybenzoic_acid (2) + K_2SO_4 (3)

Temperature: 298 K





left y-axis:

× K2SO4+4-HydroxybenzoicAcid+Water_SLE_Sugunan

○ AIOMFAC calc. SLE composition

initial weighting of dataset:

w^{init}(0904) = 1.000

dataset contribution to F_{obj}:

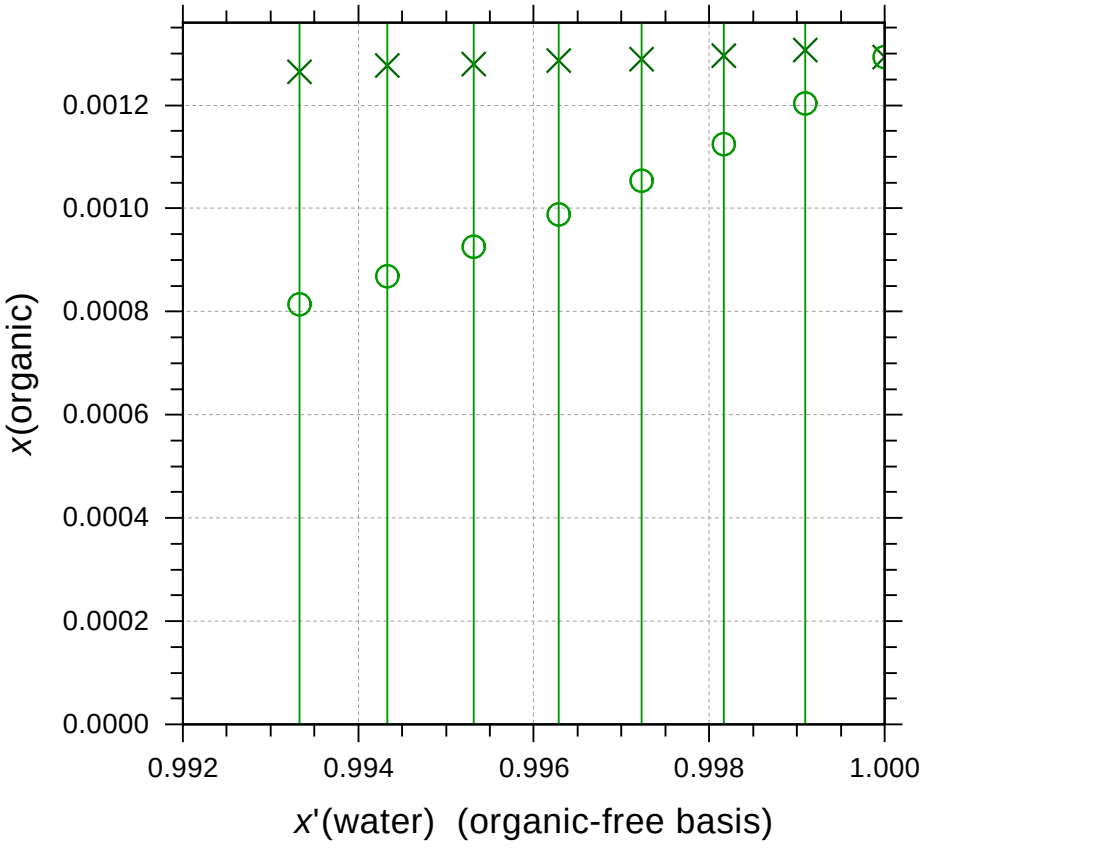
fval(0904) = 8.9220E-05

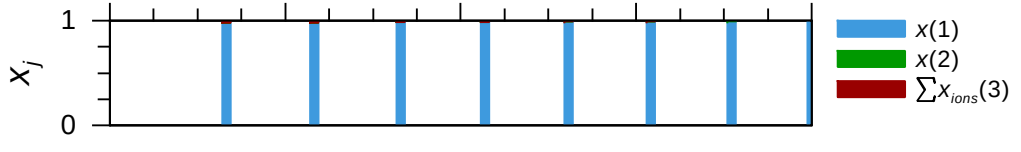
rel. contribution = 0.0000 %

Fig. S0416 (AIOMFAC_output_0908)

H_2O (1) + 4-Hydroxybenzoic_acid (2) + K_2SO_4 (3)

Temperature: 308 K



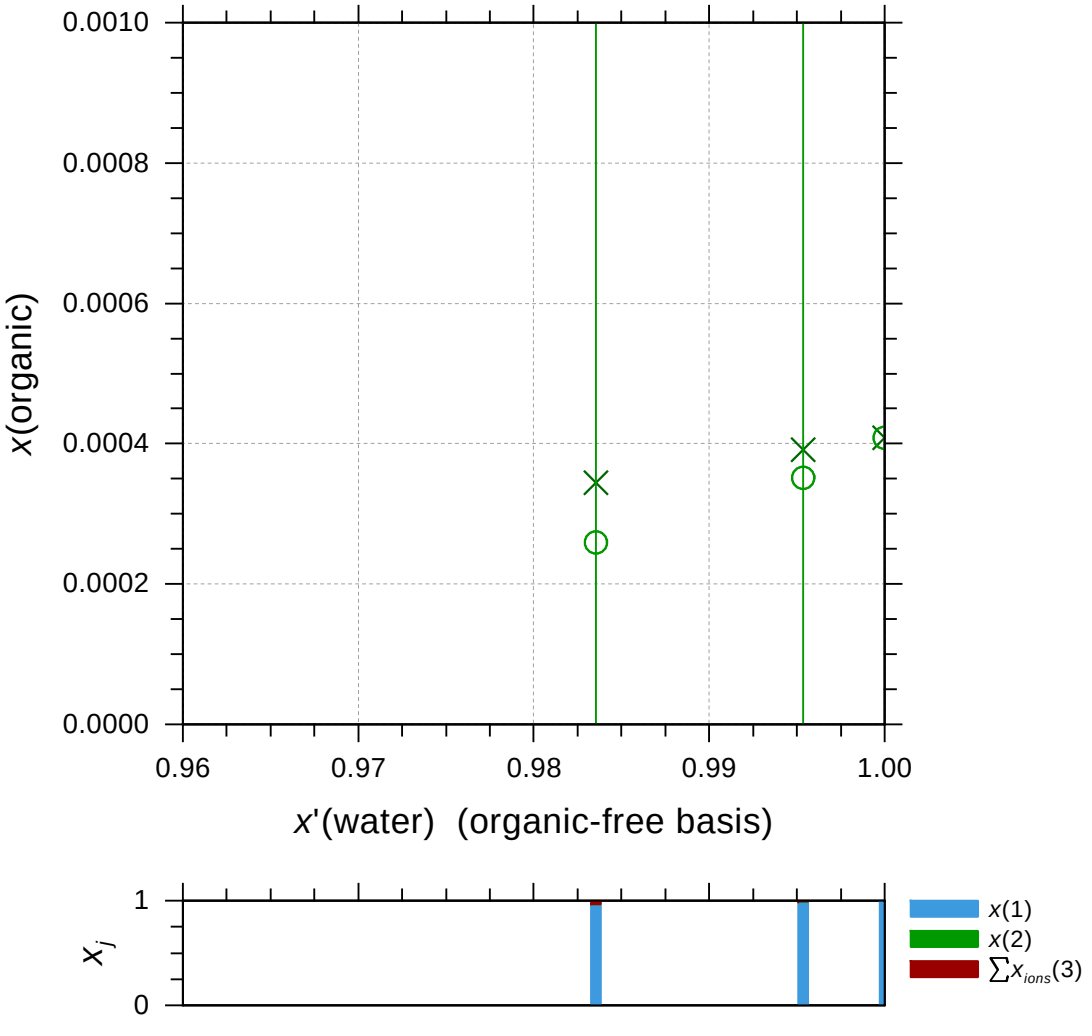


initial weighting of dataset:
w^{init}(0908) = 0.200
dataset contribution to F_{obj}:
fval(0908) = 1.0692E-03
rel. contribution = 0.0005 %

Fig. S0417 (AIOMFAC_output_0468)

H_2O (1) + Benzene (2) + KBr (3)

Temperature: 298 K

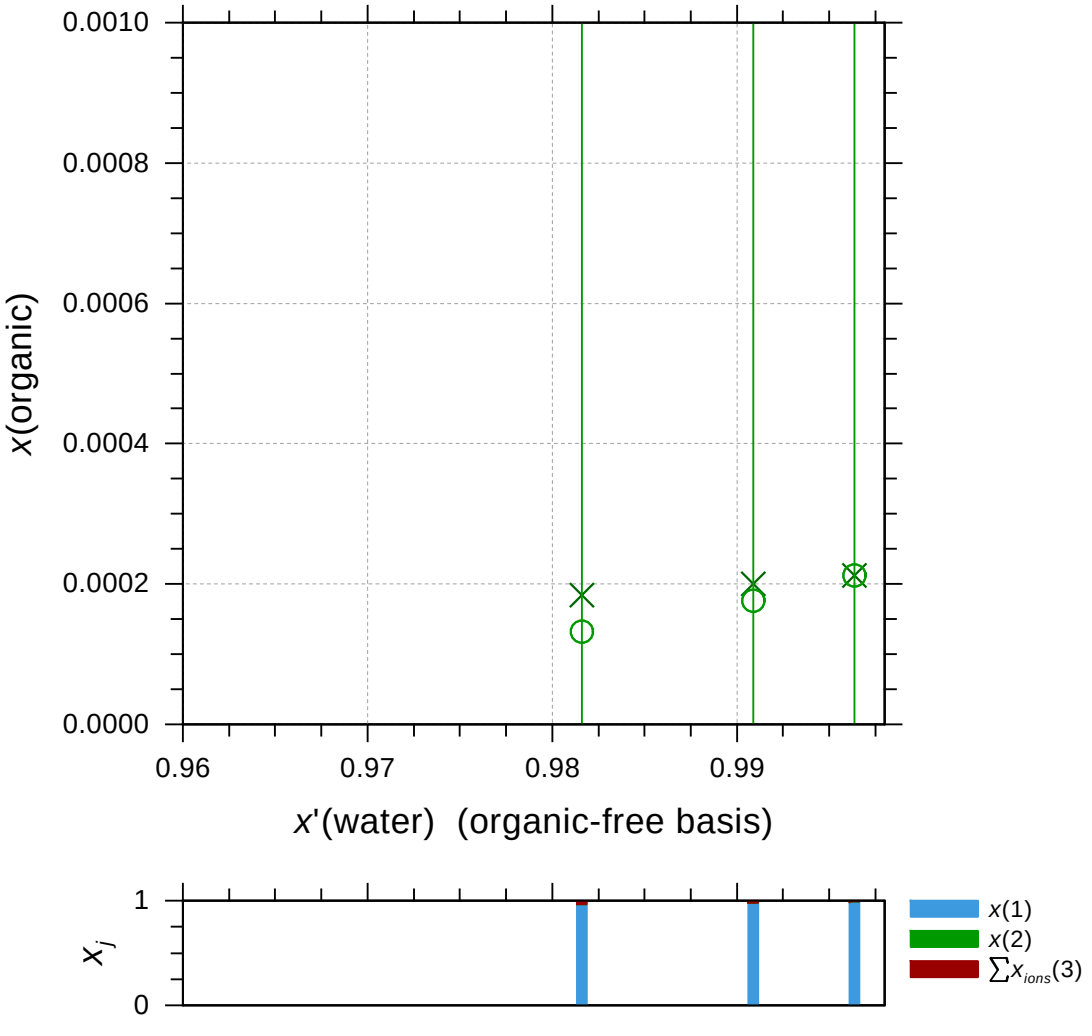


initial weighting of dataset:
w^{init}(0468) = 1.000
dataset contribution to F_{obj}:
fval(0468) = 8.1909E-05
rel. contribution = 0.0000 %

Fig. S0418 (AIOMFAC_output_0477)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + KBr (3)

Temperature: 298 K

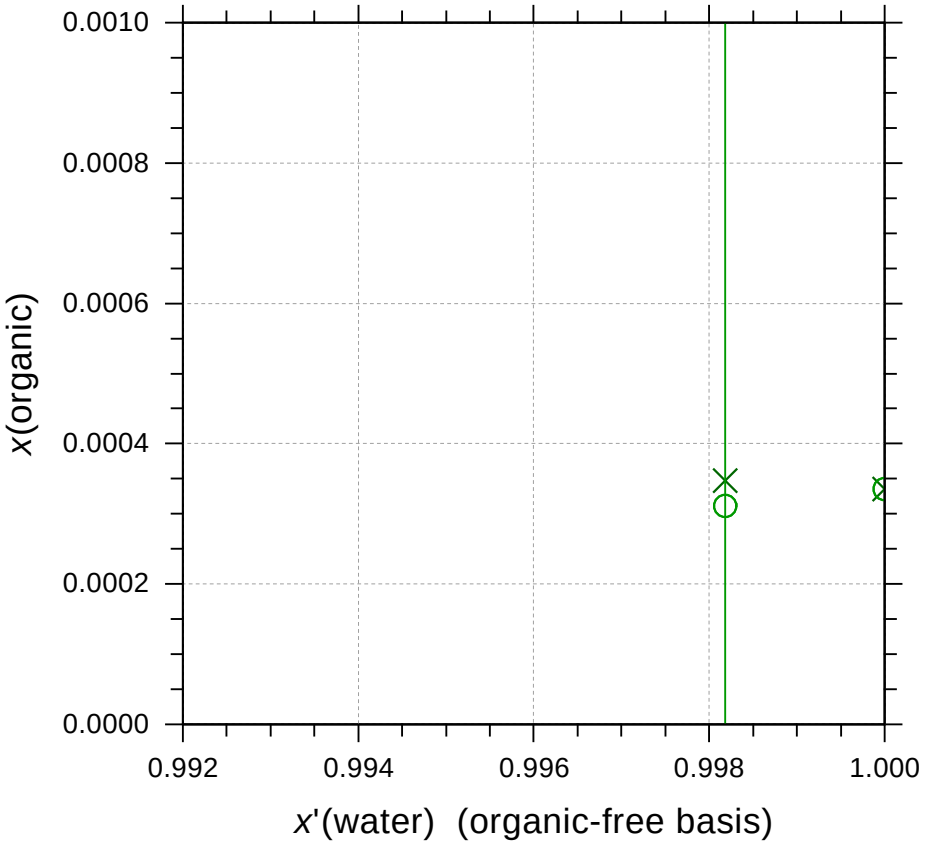


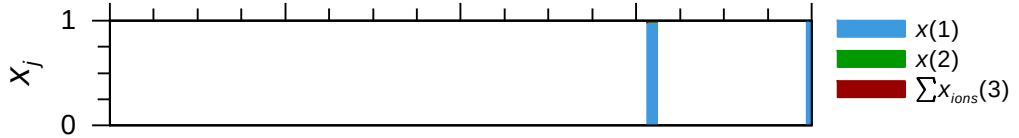
initial weighting of dataset:
$w^{init}(0477)$ = 1.000
dataset contribution to F_{obj}:
fval(0477) = 3.1734E-05
rel. contribution = 0.0000 %

Fig. S0419 (AIOMFAC_output_0492)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + KBr (3)

Temperature: 298 K



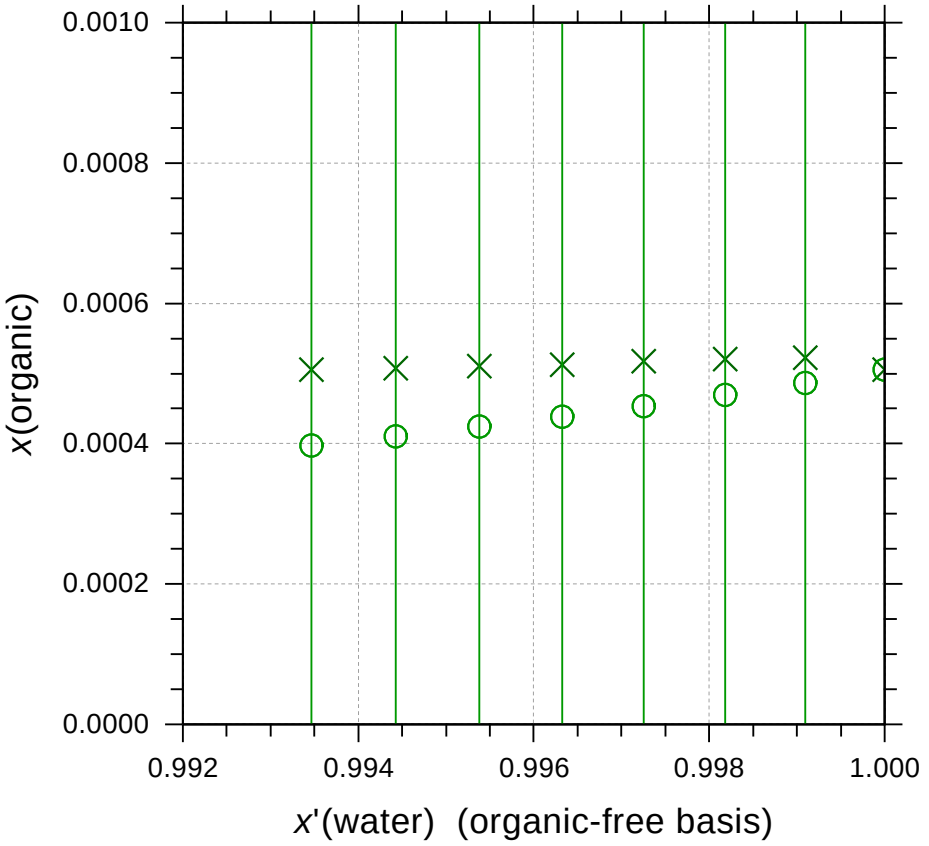


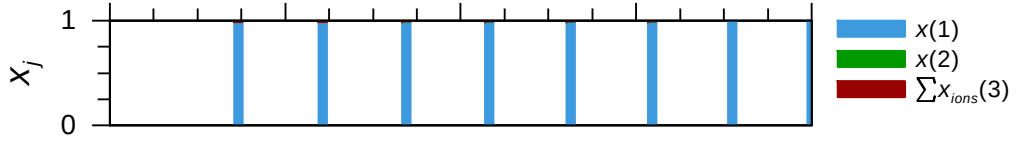
initial weighting of dataset:
w^{init}(0492) = 1.000
dataset contribution to F_{obj}:
fval(0492) = 1.2188E-05
rel. contribution = 0.0000 %

Fig. S0420 (AIOMFAC_output_0497)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + KBr (3)

Temperature: 308 K



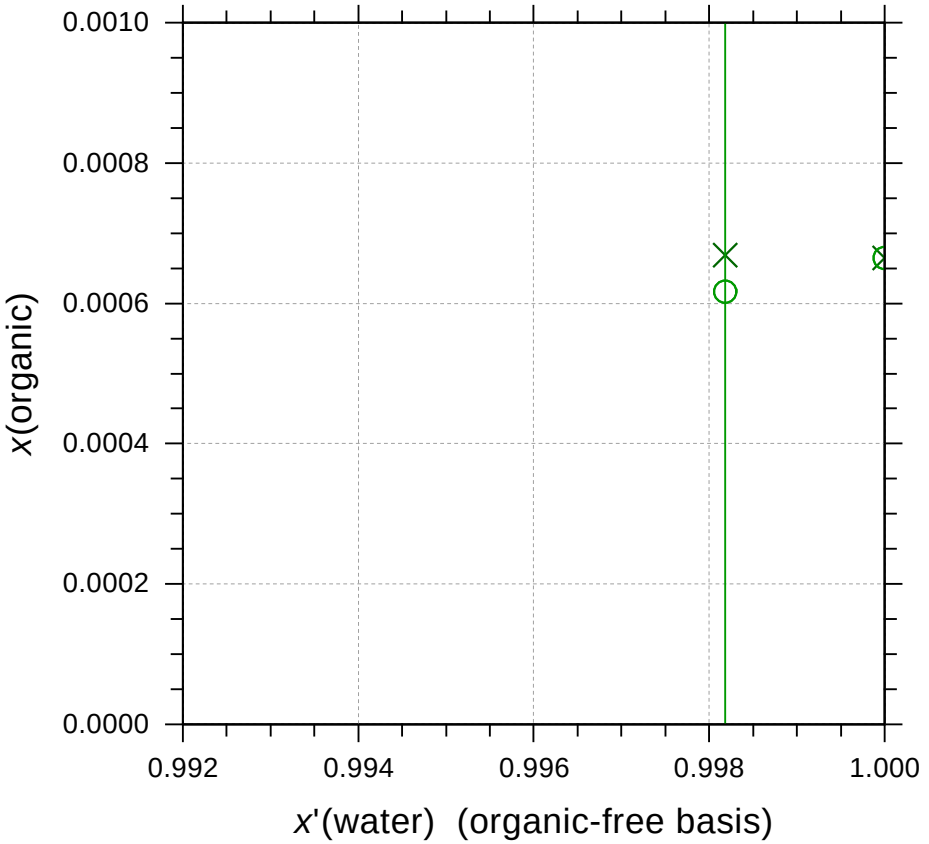


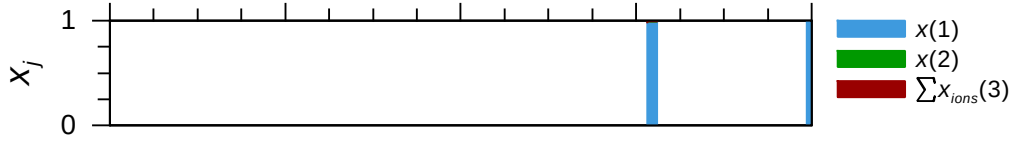
initial weighting of dataset:
w^{init}(0497) = 0.500
dataset contribution to F_{obj}:
fval(0497) = 1.9020E-04
rel. contribution = 0.0001 %

Fig. S0421 (AIOMFAC_output_0903)

H_2O (1) + 4-Hydroxybenzoic_acid (2) + KBr (3)

Temperature: 298 K





left y-axis:

× KBr+4-HydroxybenzoicAcid+Water_SLE_Sugunan

○ AIOMFAC calc. SLE composition

initial weighting of dataset:

w^{init}(0903) = 1.000

dataset contribution to F_{obj}:

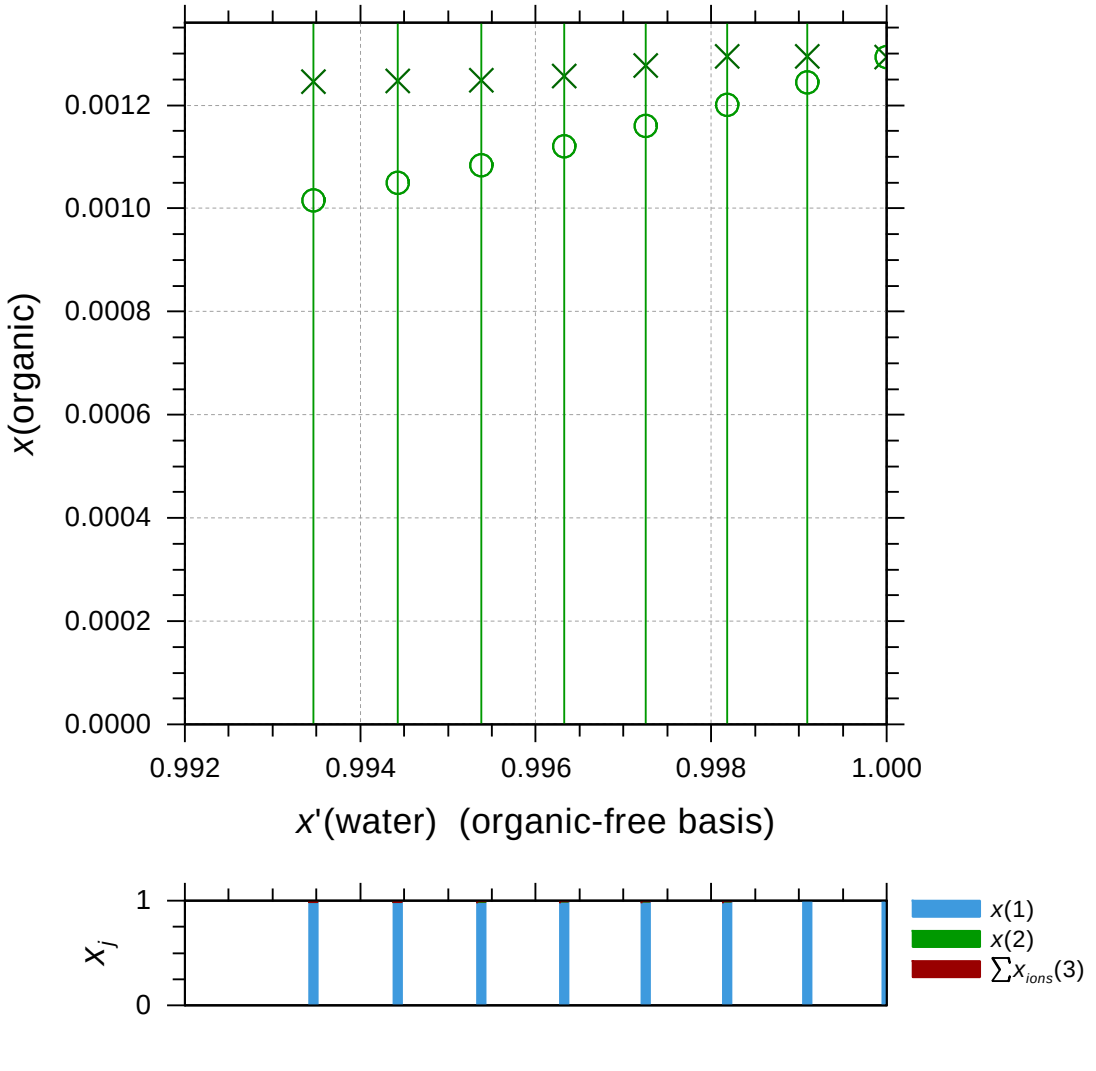
fval(0903) = 2.3031E-05

rel. contribution = 0.0000 %

Fig. S0422 (AIOMFAC_output_0907)

H_2O (1) + 4-Hydroxybenzoic_acid (2) + KBr (3)

Temperature: 308 K

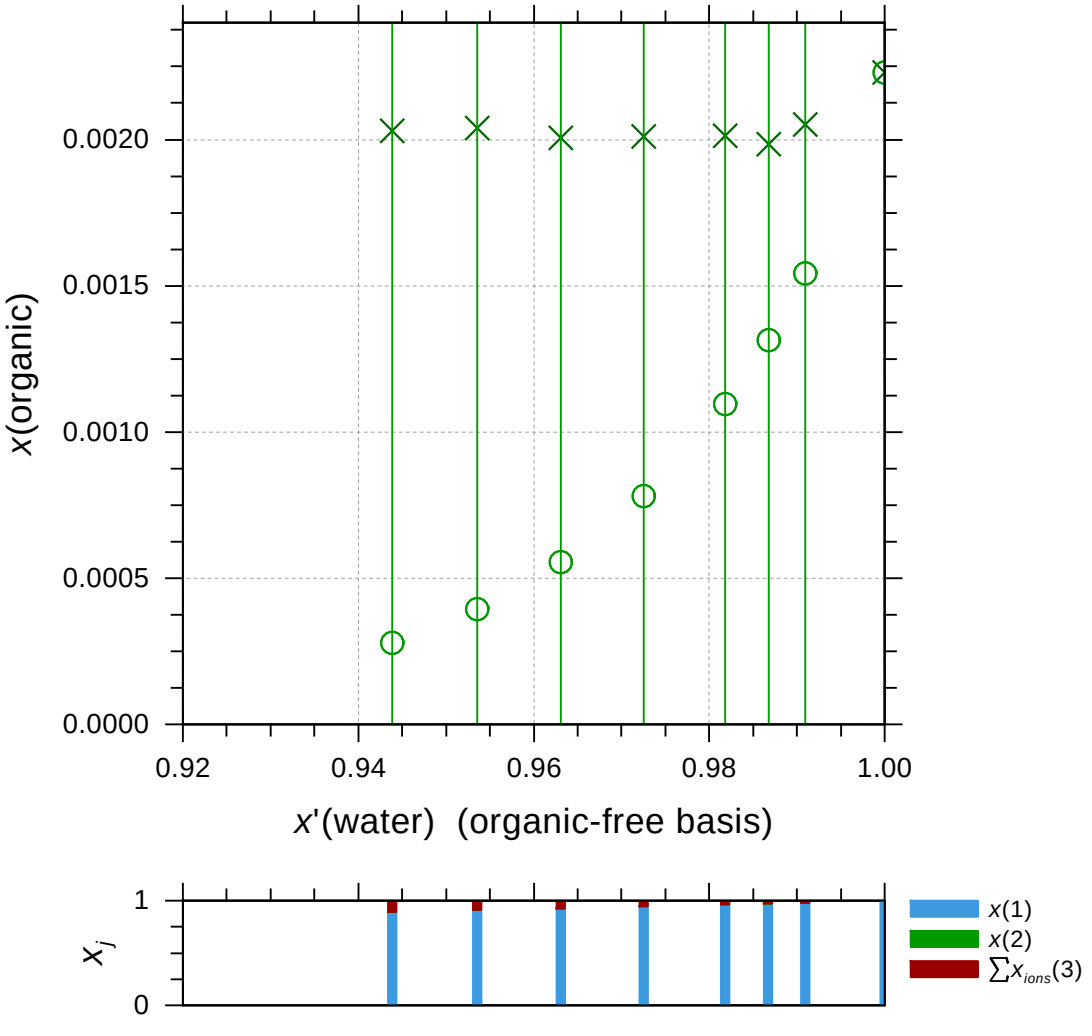


initial weighting of dataset:
$w^{init}(0907)$ = 0.500
dataset contribution to F_{obj}:
fval(0907) = 6.4150E-04
rel. contribution = 0.0003 %

Fig. S0423 (AIOMFAC_output_0445)

H_2O (1) + Protocatechuic_acid (2) + KCl (3)

Temperature: 298 K

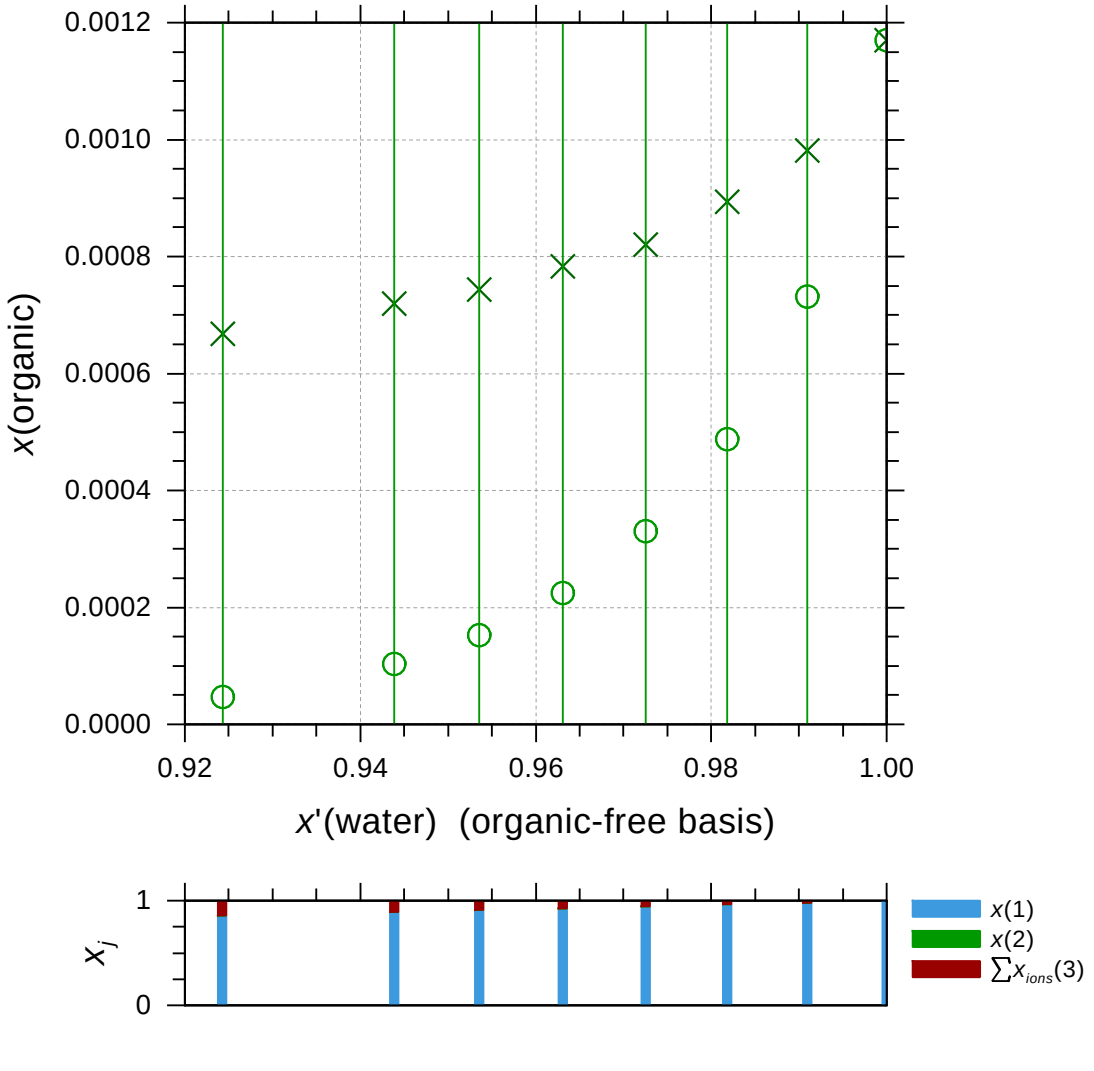


initial weighting of dataset:
w^{init}(0445) = 1.000
dataset contribution to F_{obj}:
fval(0445) = 7.5824E-02
rel. contribution = 0.0361 %

Fig. S0424 (AIOMFAC_output_0448)

H_2O (1) + Vanillin (2) + KCl (3)

Temperature: 298 K

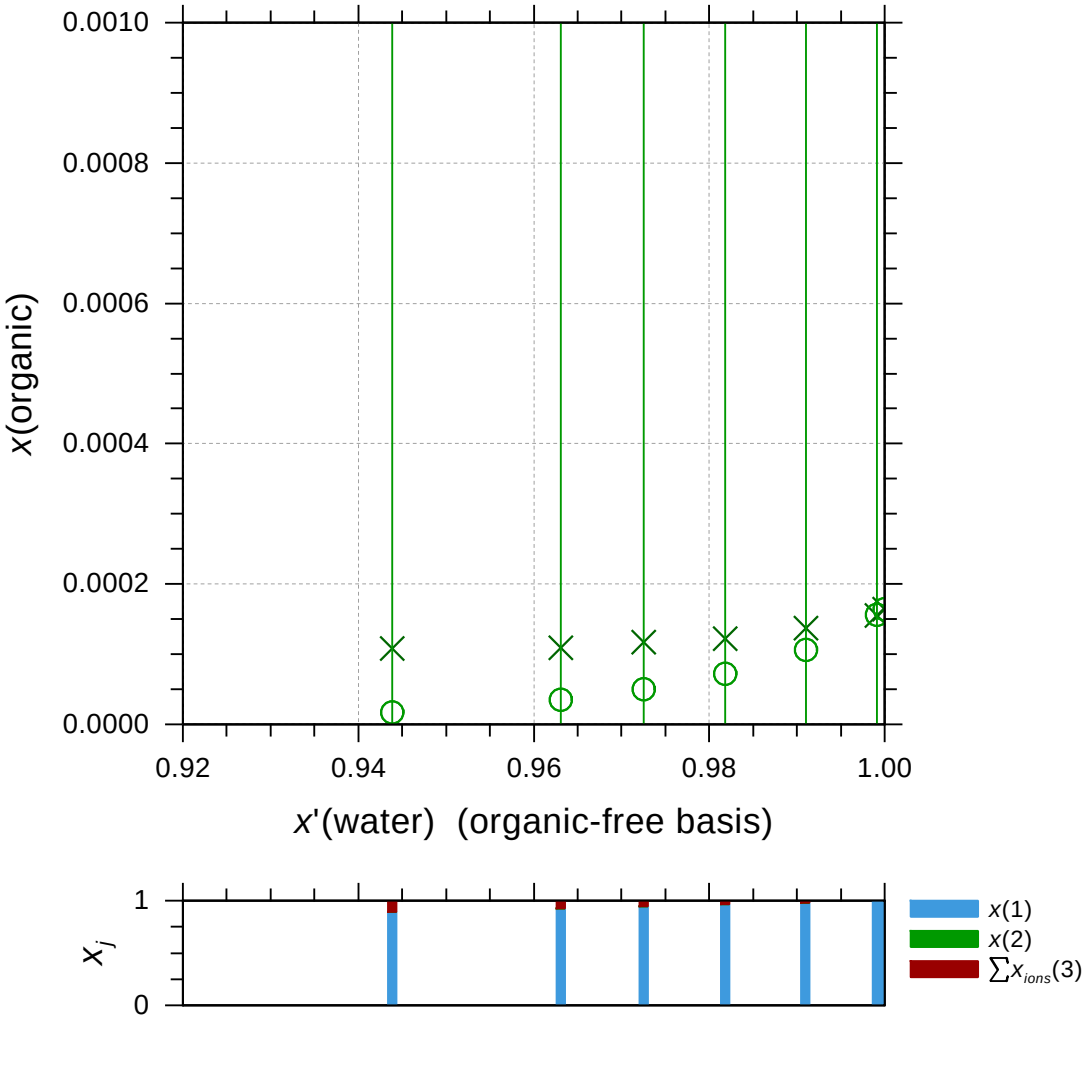


initial weighting of dataset:
w^{init}(0448) = 1.000
dataset contribution to F_{obj}:
fval(0448) = 1.6363E-02
rel. contribution = 0.0078 %

Fig. S0425 (AIOMFAC_output_0451)

H_2O (1) + Vanillic_acid (2) + KCl (3)

Temperature: 298 K

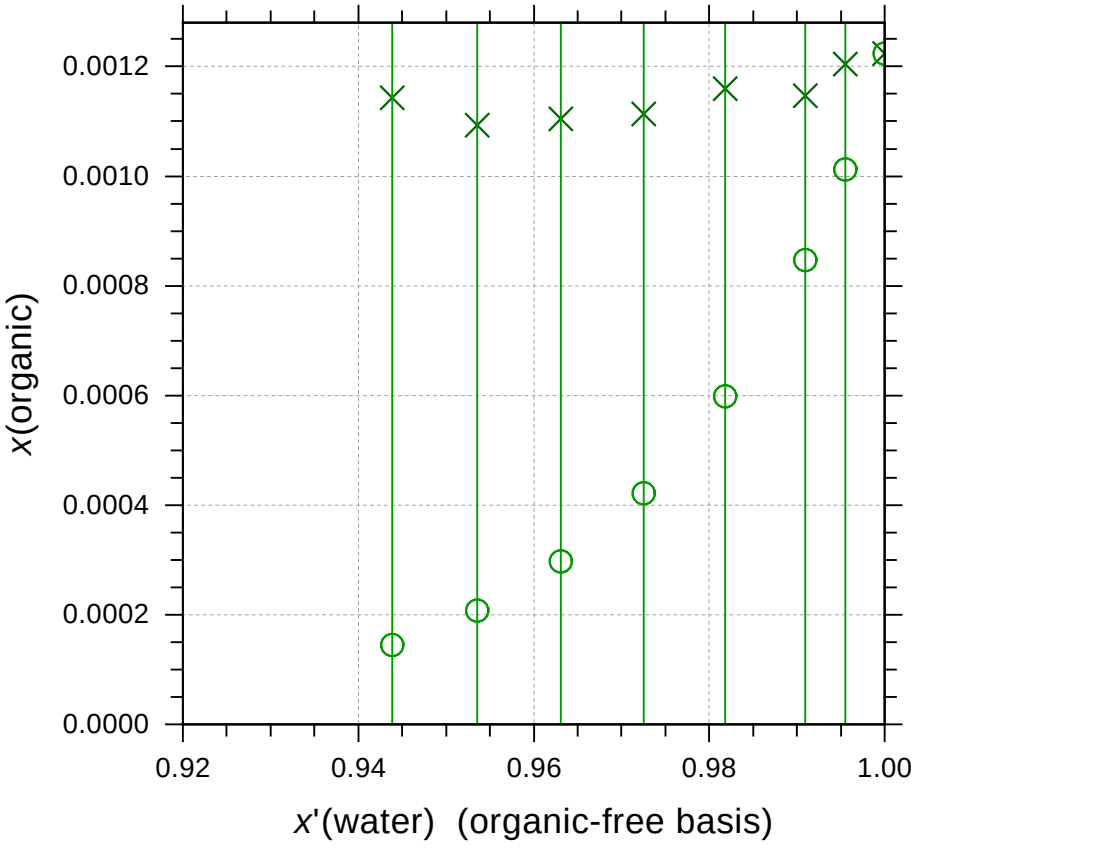


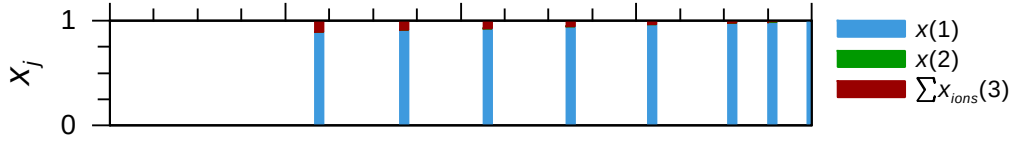
initial weighting of dataset:
$w^{init}(0451)$ = 1.000
dataset contribution to F_{obj}:
fval(0451) = 2.1353E-04
rel. contribution = 0.0001 %

Fig. S0426 (AIOMFAC_output_0454)

H_2O (1) + Gallic_acid (2) + KCl (3)

Temperature: 298 K



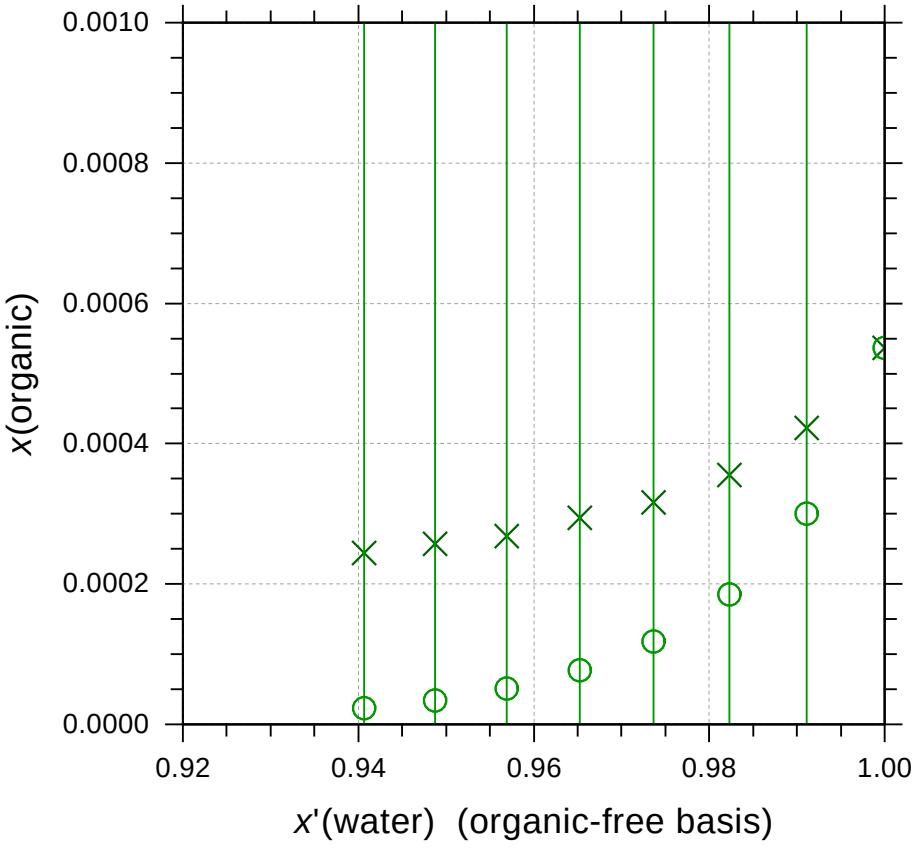


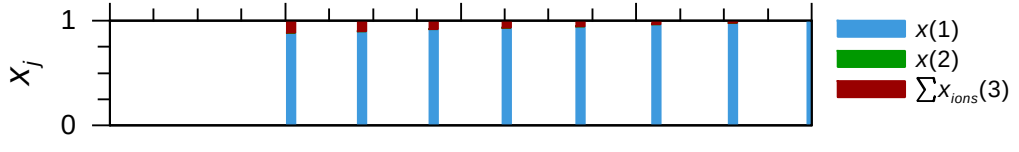
initial weighting of dataset:
w^{init}(0454) = 1.000
dataset contribution to F_{obj}:
fval(0454) = 2.7099E-02
rel. contribution = 0.0129 %

Fig. S0427 (AIOMFAC_output_0457)

H_2O (1) + Ferulic_acid (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl+FerulicAcid+Water_SLE_Noubigh

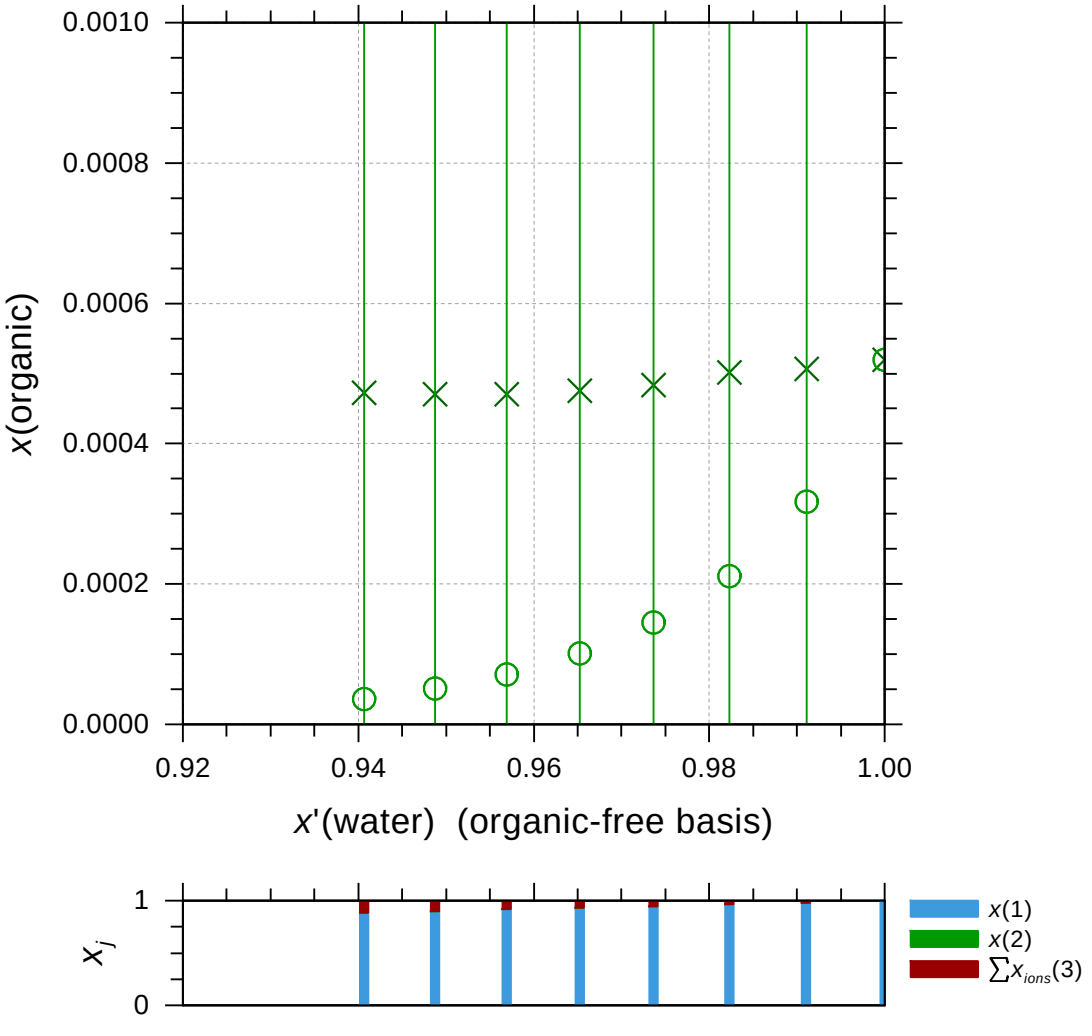
○ AIOMFAC calc. SLE composition

initial weighting of dataset:
w^{init}(0457) = 1.000
dataset contribution to F_{obj}:
fval(0457) = 2.5980E-03
rel. contribution = 0.0012 %

Fig. S0428 (AIOMFAC_output_0460)

H_2O (1) + Syringic_acid (2) + KCl (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0460)$ = 1.000

dataset contribution to F_{obj}:

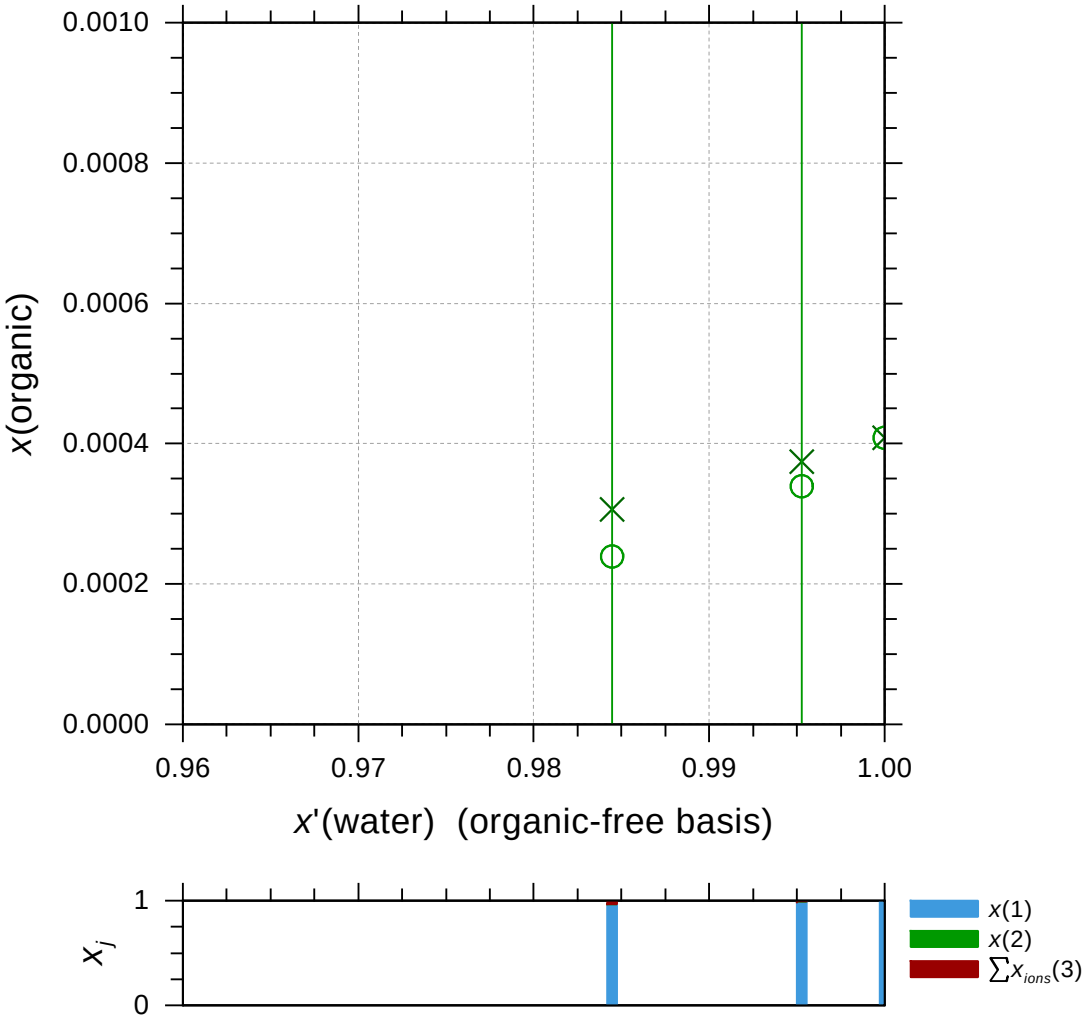
fval(0460) = 8.1902E-03

rel. contribution = 0.0039 %

Fig. S0429 (AIOMFAC_output_0467)

H_2O (1) + Benzene (2) + KCl (3)

Temperature: 298 K

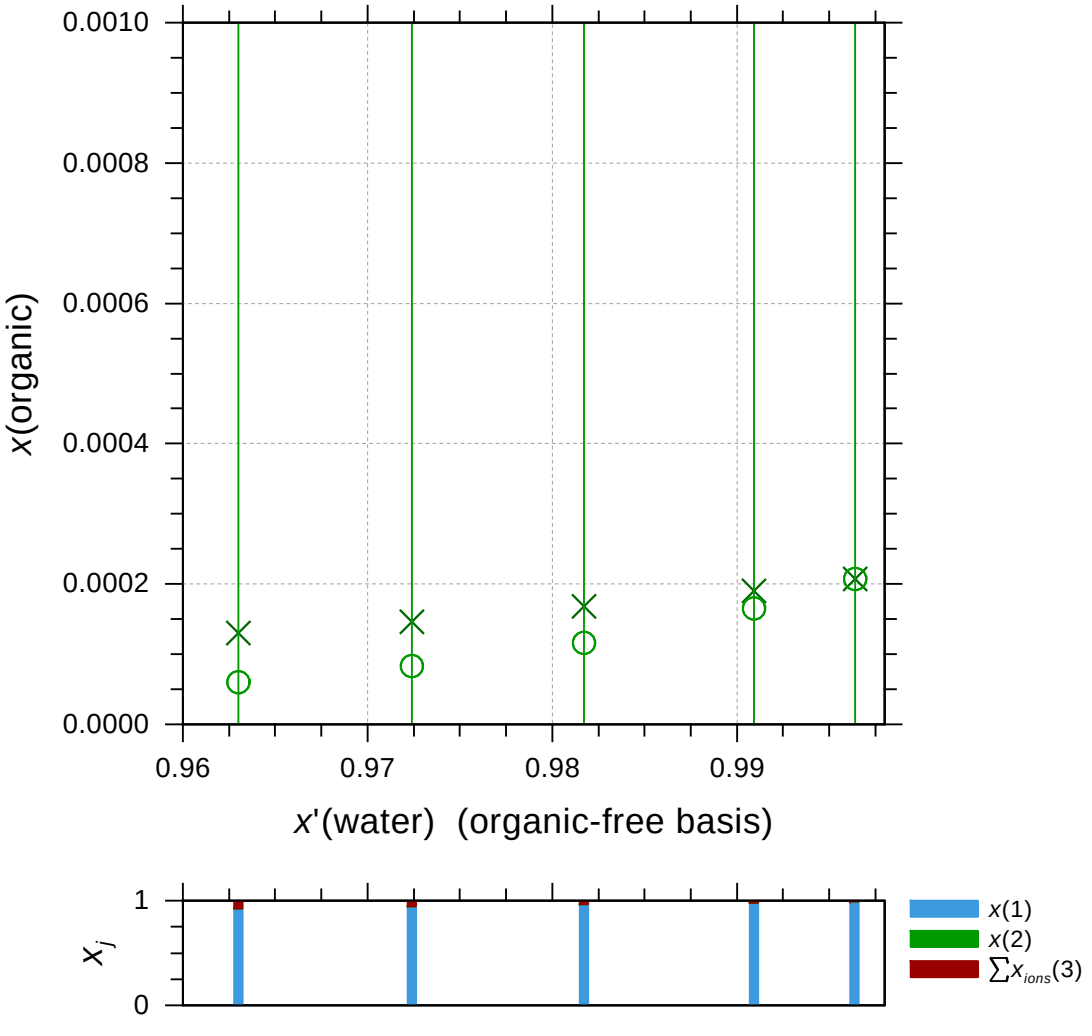


initial weighting of dataset:
w^{init}(0467) = 1.000
dataset contribution to F_{obj}:
fval(0467) = 5.3692E-05
rel. contribution = 0.0000 %

Fig. S0430 (AIOMFAC_output_0472)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + KCl (3)

Temperature: 298 K



initial weighting of dataset:

w^{init}(0472) = 1.000

dataset contribution to F_{obj}:

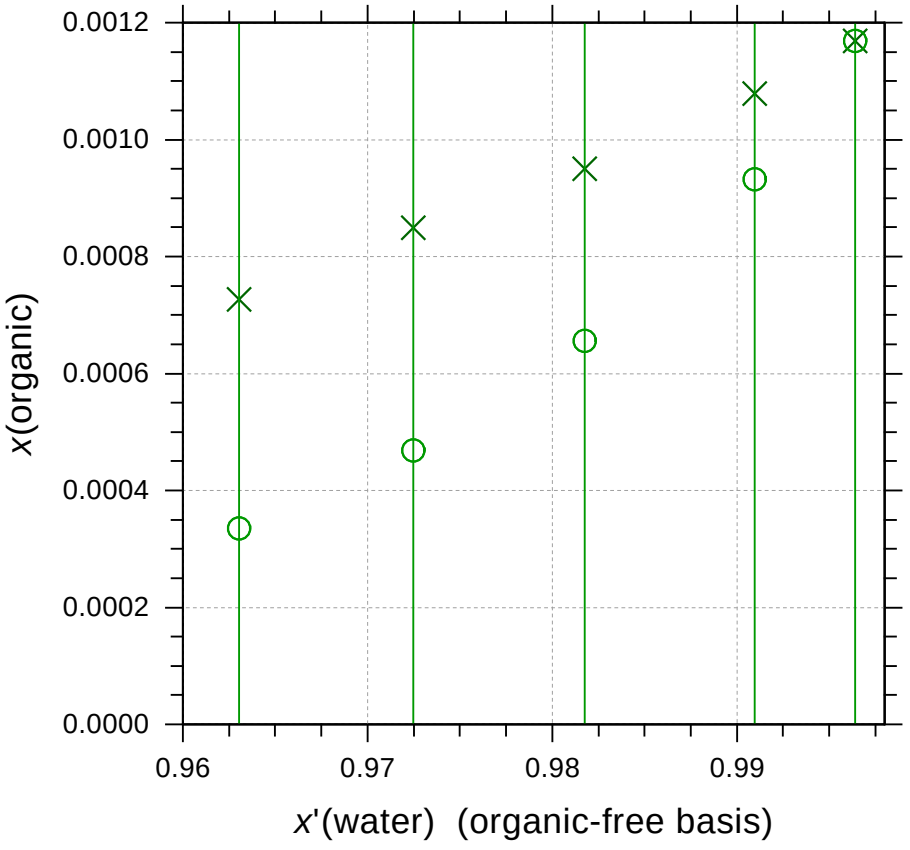
fval(0472) = 1.1964E-04

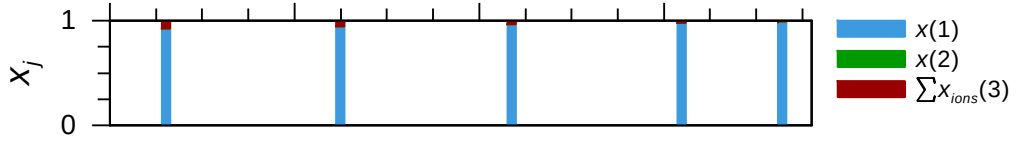
rel. contribution = 0.0001 %

Fig. S0431 (AIOMFAC_output_0473)

H_2O (1) + 3-Hydroxybenzoic_acid (2) + KCl (3)

Temperature: 298 K



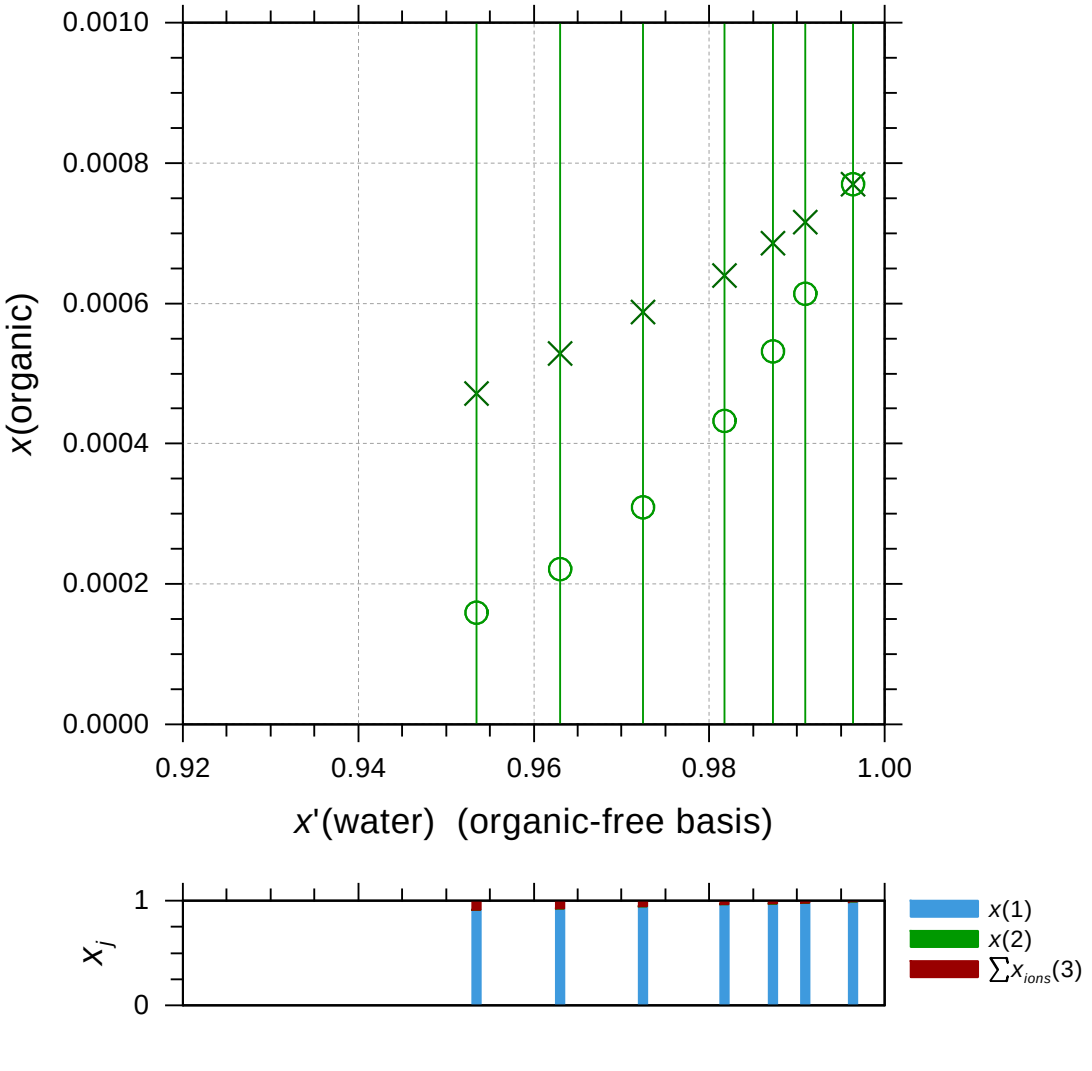


initial weighting of dataset:
w^{init}(0473) = 1.000
dataset contribution to F_{obj}:
fval(0473) = 3.4574E-03
rel. contribution = 0.0016 %

Fig. S0432 (AIOMFAC_output_0474)

H_2O (1) + 4-Hydroxybenzoic_acid (2) + KCl (3)

Temperature: 298 K

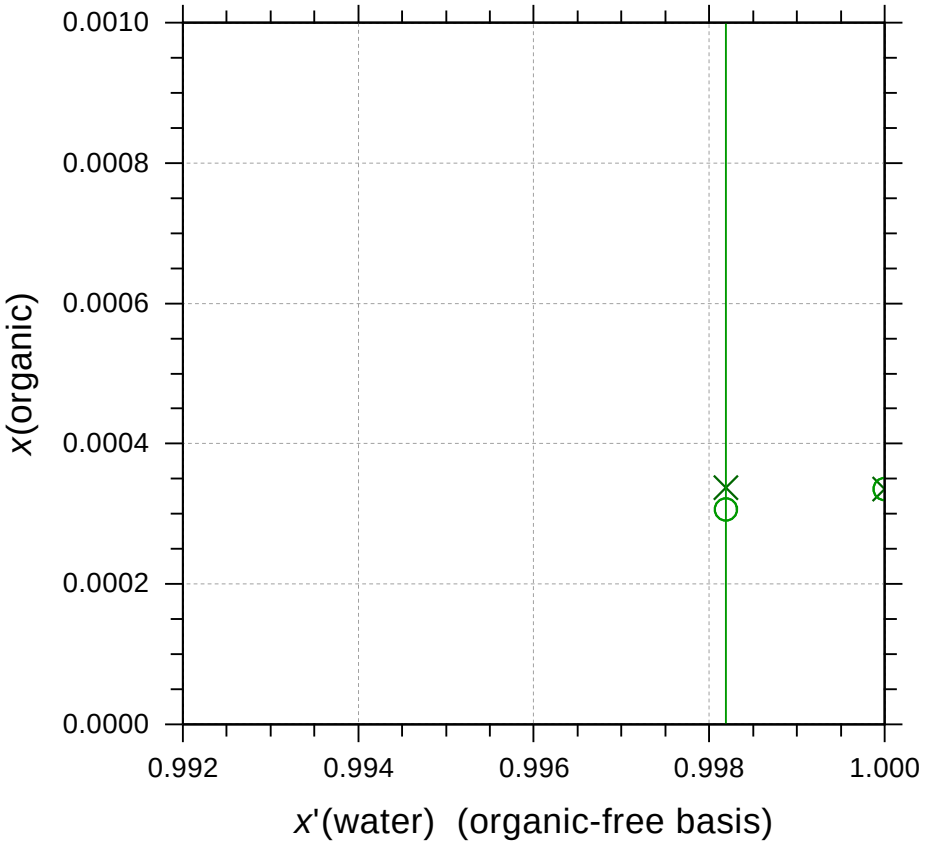


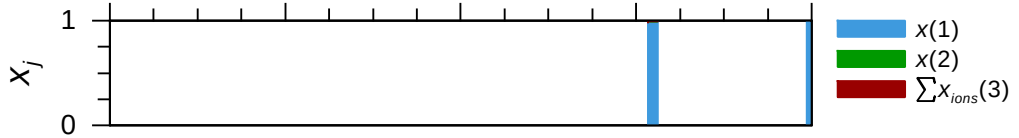
initial weighting of dataset:
$w^{init}(0474)$ = 1.000
dataset contribution to F_{obj}:
fval(0474) = 3.1128E-03
rel. contribution = 0.0015 %

Fig. S0433 (AIOMFAC_output_0491)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + KCl (3)

Temperature: 298 K



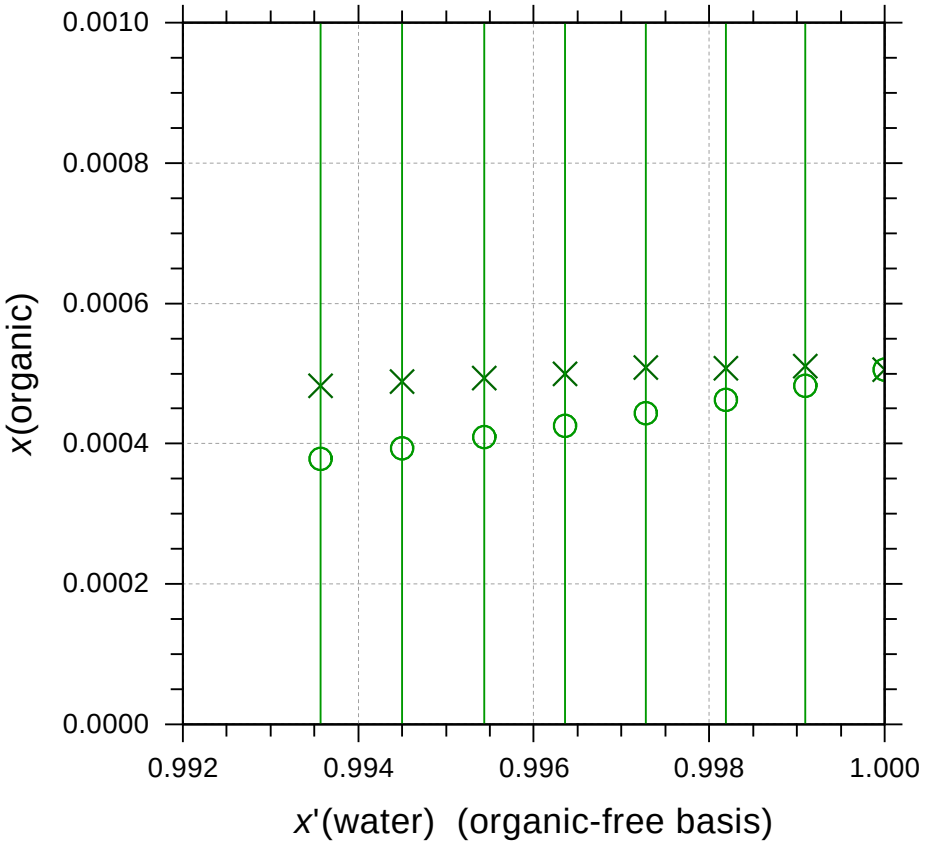


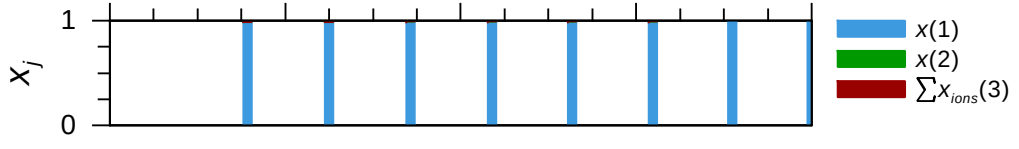
initial weighting of dataset:
w^{init}(0491) = 1.000
dataset contribution to F_{obj}:
fval(0491) = 8.7889E-06
rel. contribution = 0.0000 %

Fig. S0434 (AIOMFAC_output_0496)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + KCl (3)

Temperature: 308 K



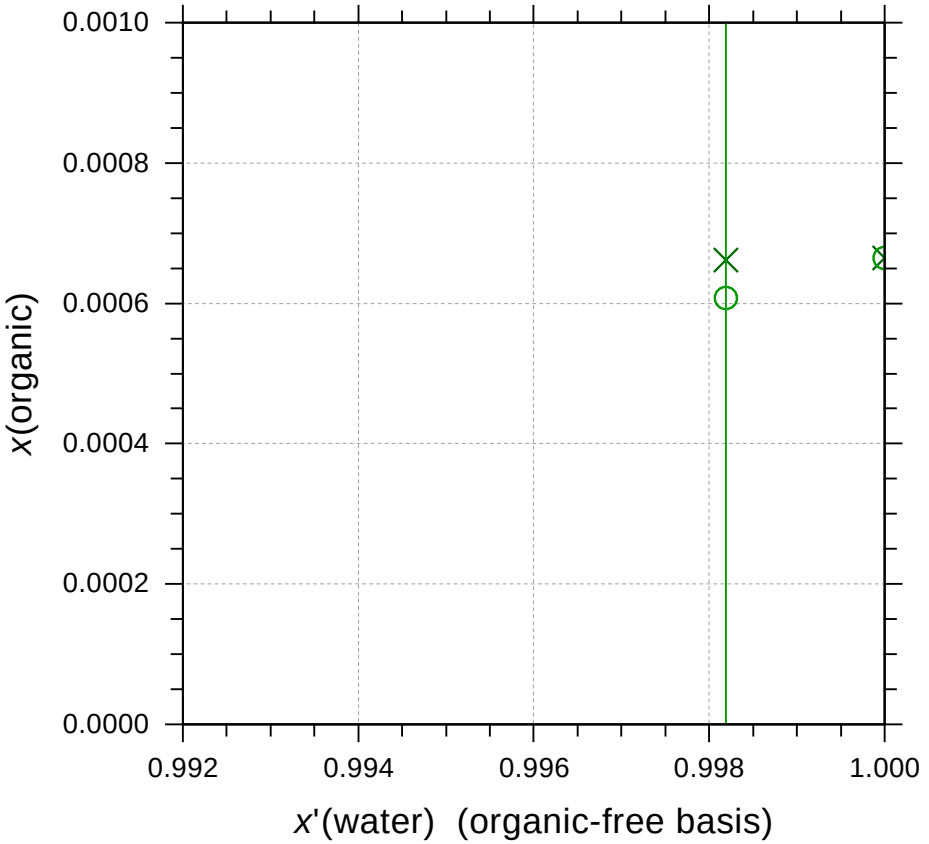


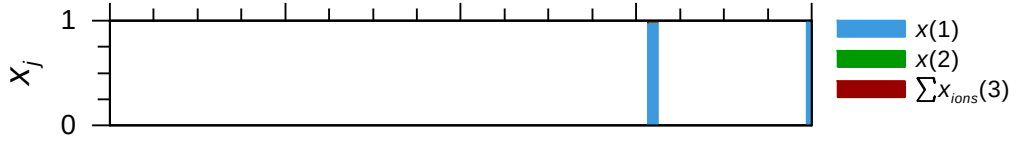
initial weighting of dataset:
w^{init}(0496) = 0.500
dataset contribution to F_{obj}:
fval(0496) = 1.7907E-04
rel. contribution = 0.0001 %

Fig. S0435 (AIOMFAC_output_0902)

H_2O (1) + 4-Hydroxybenzoic_acid (2) + KCl (3)

Temperature: 298 K





left y-axis:

× KCl+4-HydroxybenzoicAcid+Water_SLE_Sugunan

○ AIOMFAC calc. SLE composition

initial weighting of dataset:

w^{init}(0902) = 1.000

dataset contribution to F_{obj}:

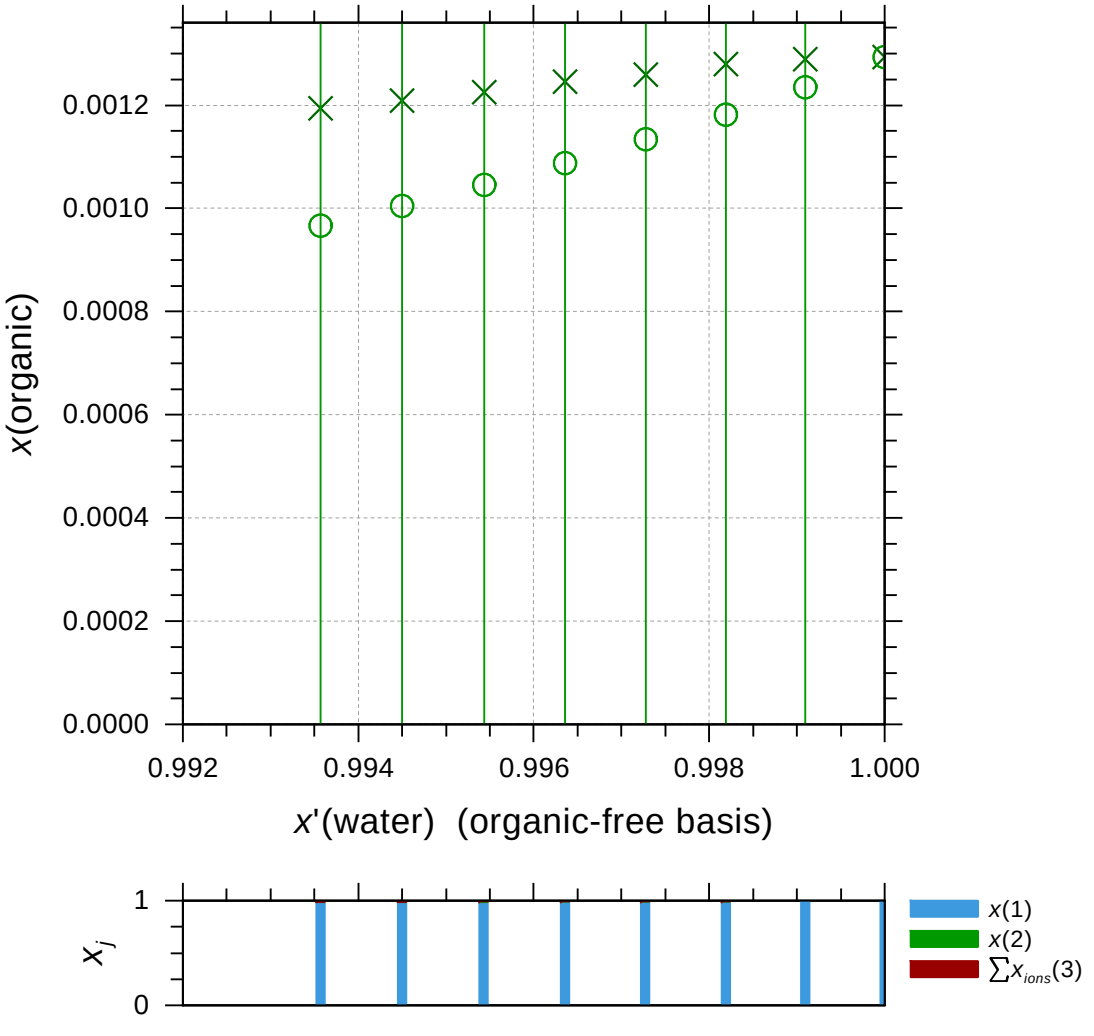
fval(0902) = 2.5389E-05

rel. contribution = 0.0000 %

Fig. S0436 (AIOMFAC_output_0906)

H_2O (1) + 4-Hydroxybenzoic_acid (2) + KCl (3)

Temperature: 308 K

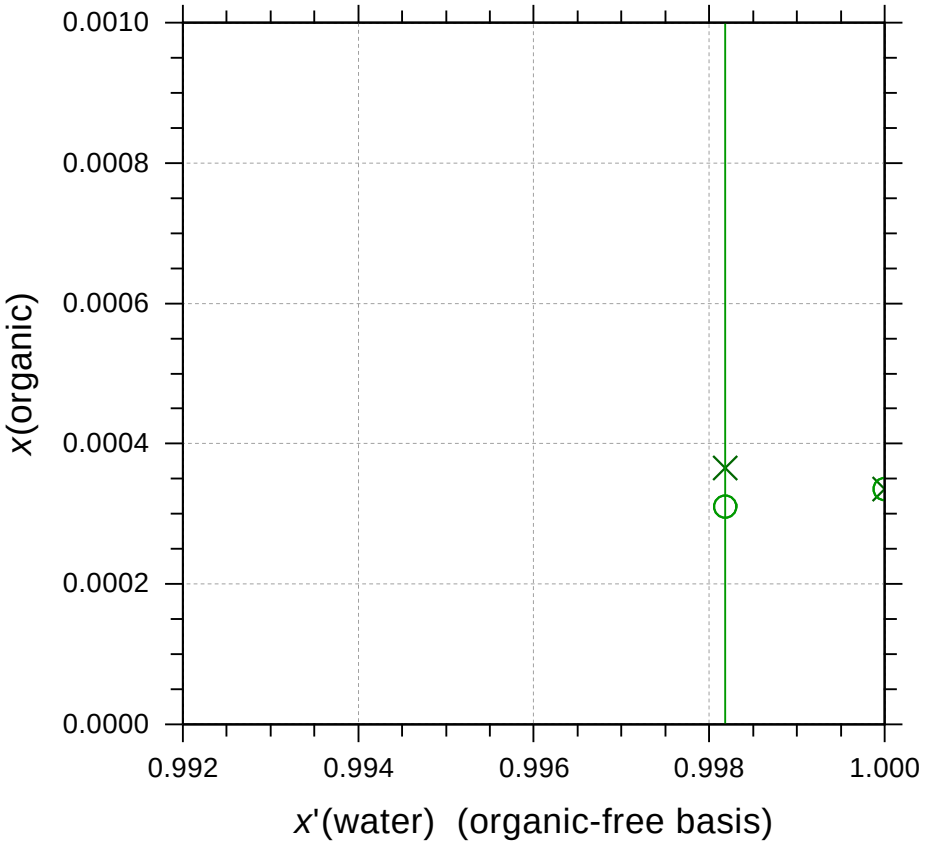


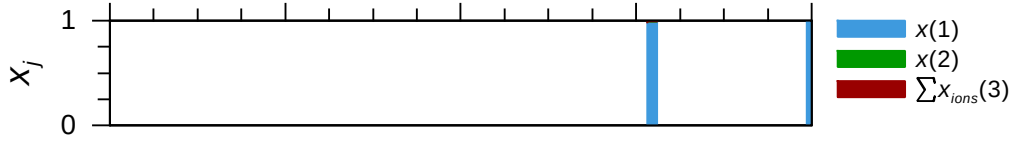
initial weighting of dataset:
$w^{init}(0906)$ = 0.500
dataset contribution to F_{obj}:
fval(0906) = 7.0663E-04
rel. contribution = 0.0003 %

Fig. S0437 (AIOMFAC_output_0493)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + KNO_3 (3)

Temperature: 298 K





left y-axis:

× KNO3+2-HydroxybenzoicAcid+Water_SLE_Sugunan

○ AIOMFAC calc. SLE composition

initial weighting of dataset:

w^{init}(0493) = 1.000

dataset contribution to F_{obj}:

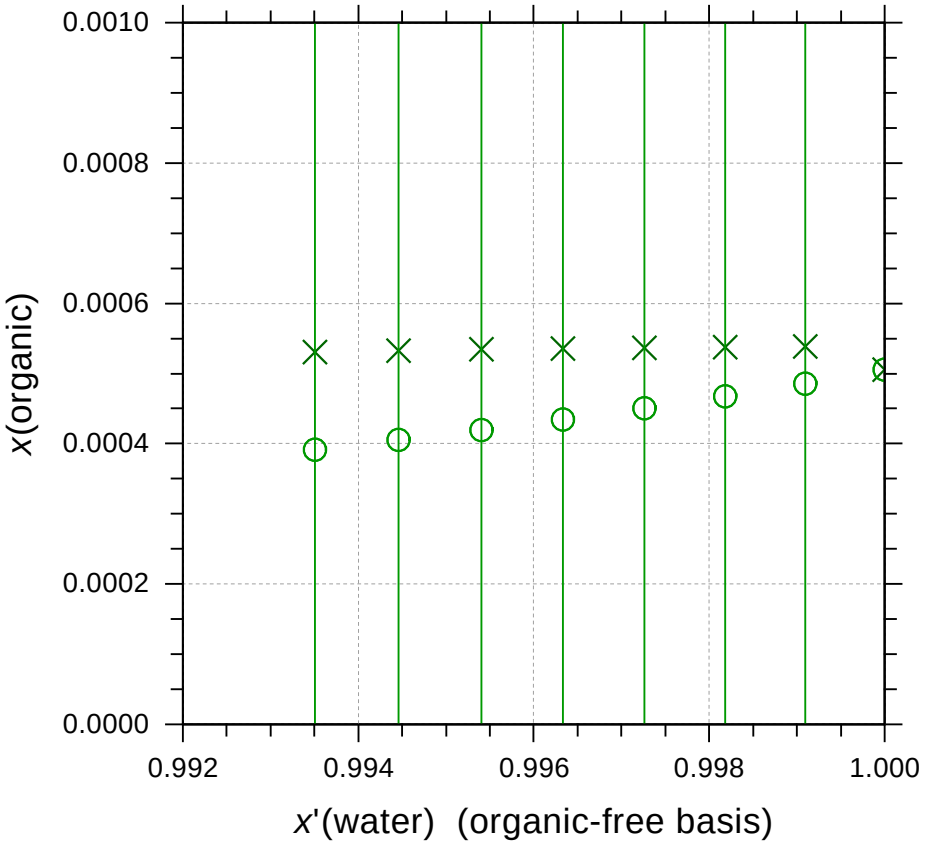
fval(0493) = 2.7986E-05

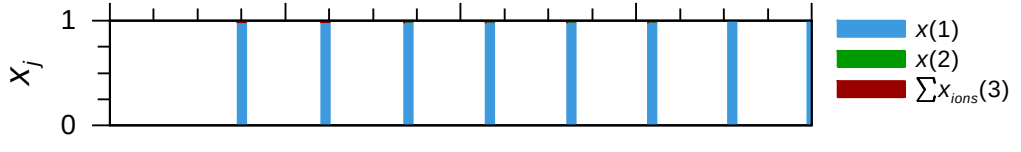
rel. contribution = 0.0000 %

Fig. S0438 (AIOMFAC_output_0498)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + KNO_3 (3)

Temperature: 308 K





left y-axis:

× KNO3+2-HydroxybenzoicAcid+Water_SLE_308K_Sugunan

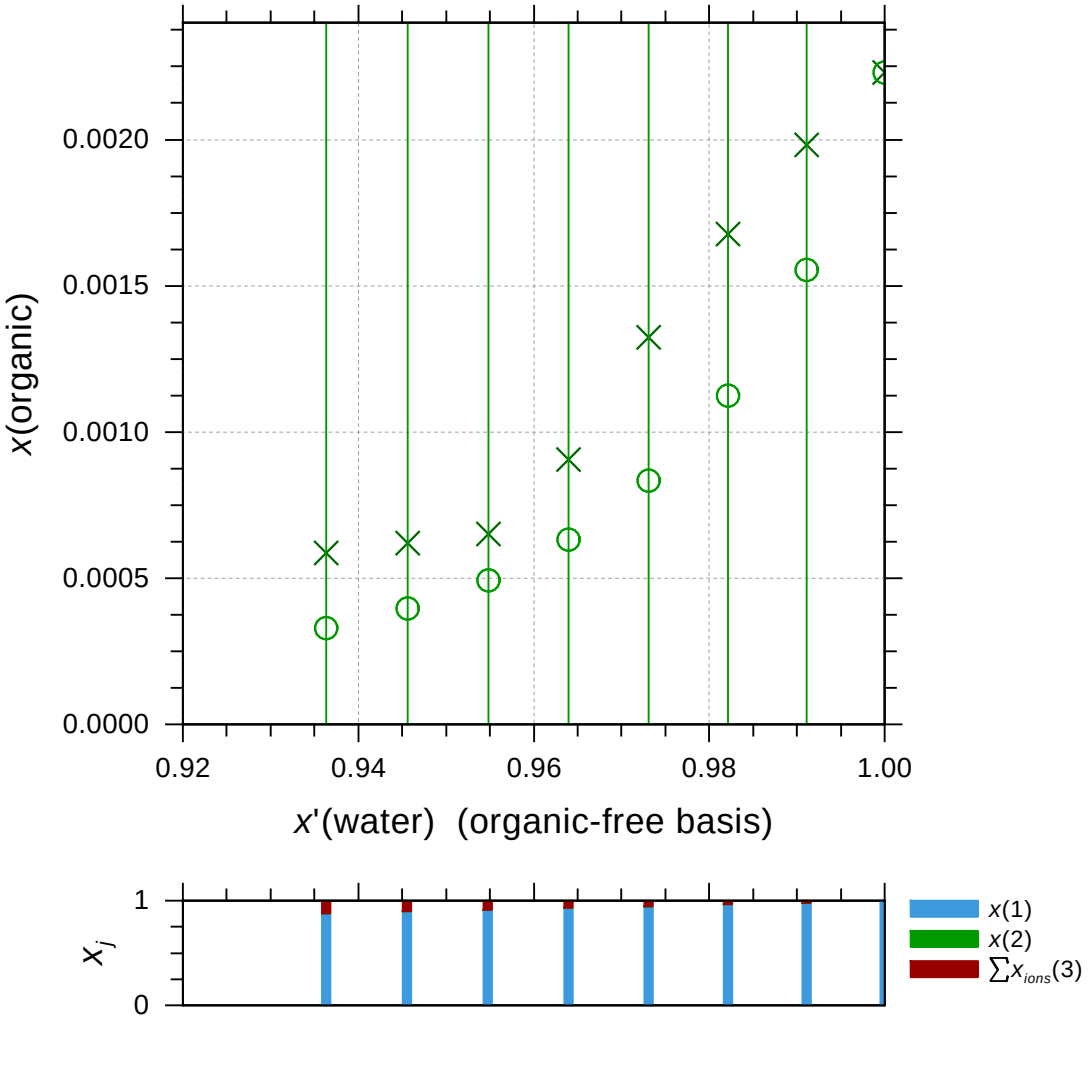
○ AIOMFAC calc. SLE composition

initial weighting of dataset:
w^{init}(0498) = 0.500
dataset contribution to F_{obj}:
fval(0498) = 3.3287E-04
rel. contribution = 0.0002 %

Fig. S0439 (AIOMFAC_output_0447)

H_2O (1) + Protocatechuic_acid (2) + LiCl (3)

Temperature: 298 K

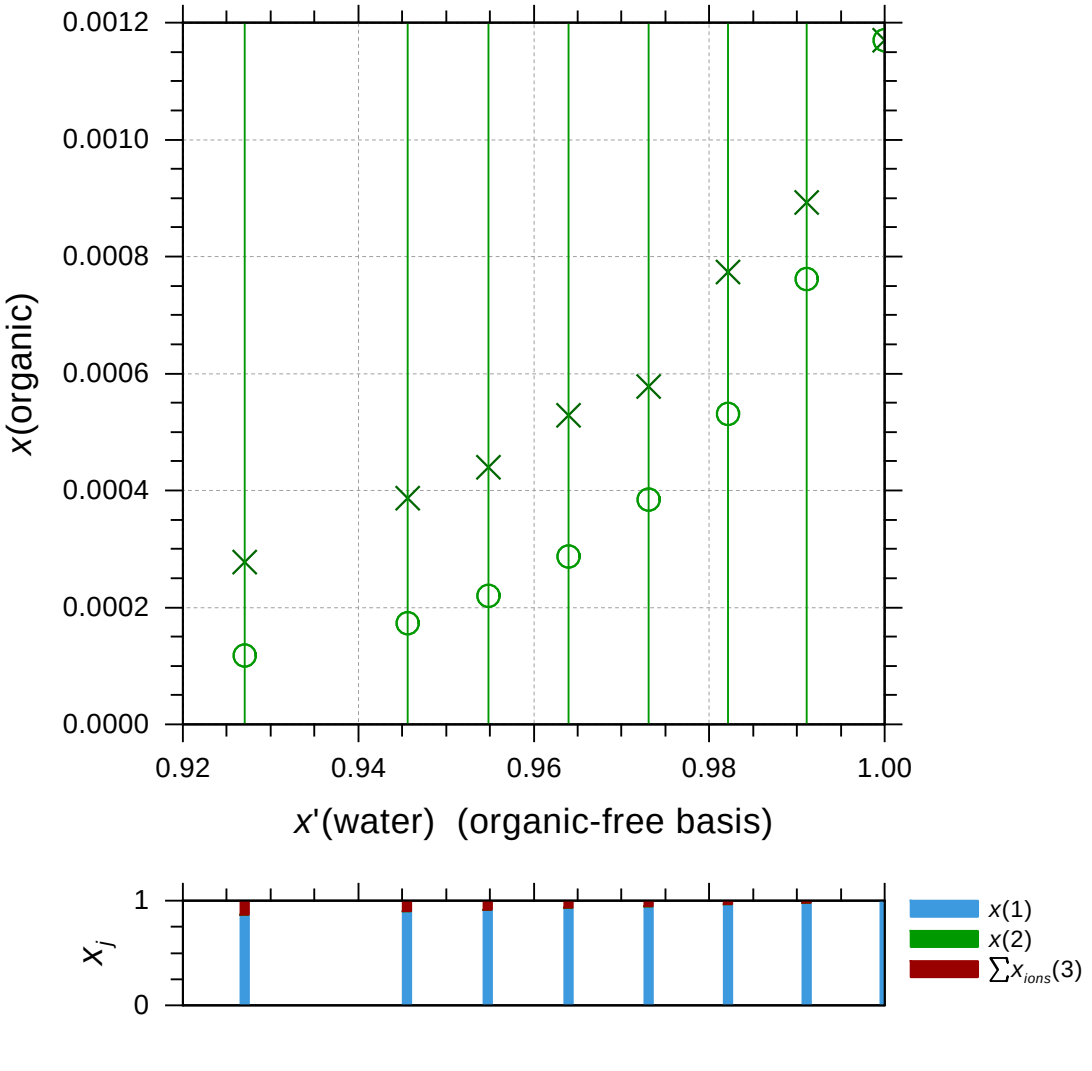


initial weighting of dataset:
w^{init}(0447) = 1.000
dataset contribution to F_{obj}:
fval(0447) = 7.2814E-03
rel. contribution = 0.0035 %

Fig. S0440 (AIOMFAC_output_0450)

H_2O (1) + Vanillin (2) + LiCl (3)

Temperature: 298 K



initial weighting of dataset:

w^{init}(0450) = 1.000

dataset contribution to F_{obj}:

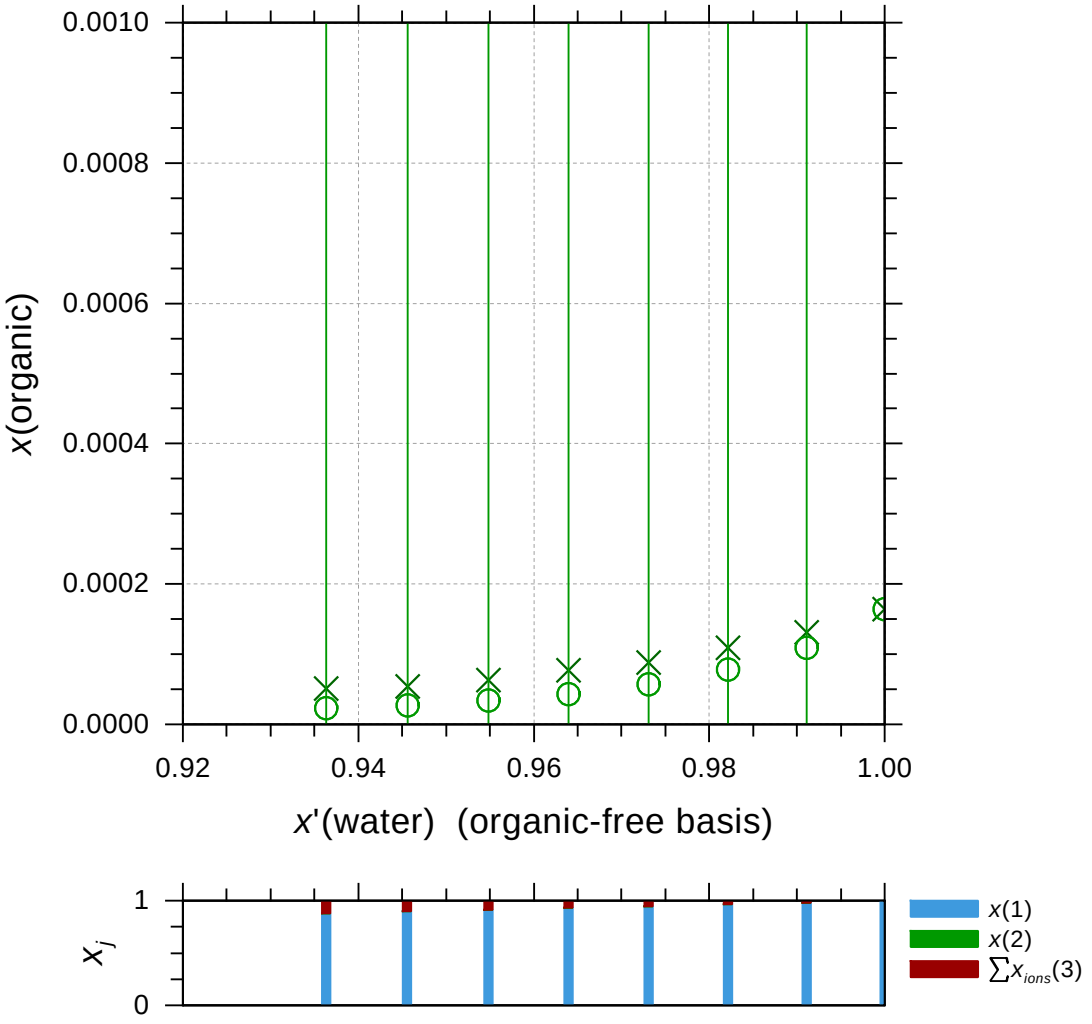
fval(0450) = 2.6254E-03

rel. contribution = 0.0012 %

Fig. S0441 (AIOMFAC_output_0453)

H_2O (1) + Vanillic_acid (2) + LiCl (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0453)$ = 1.000

dataset contribution to F_{obj}:

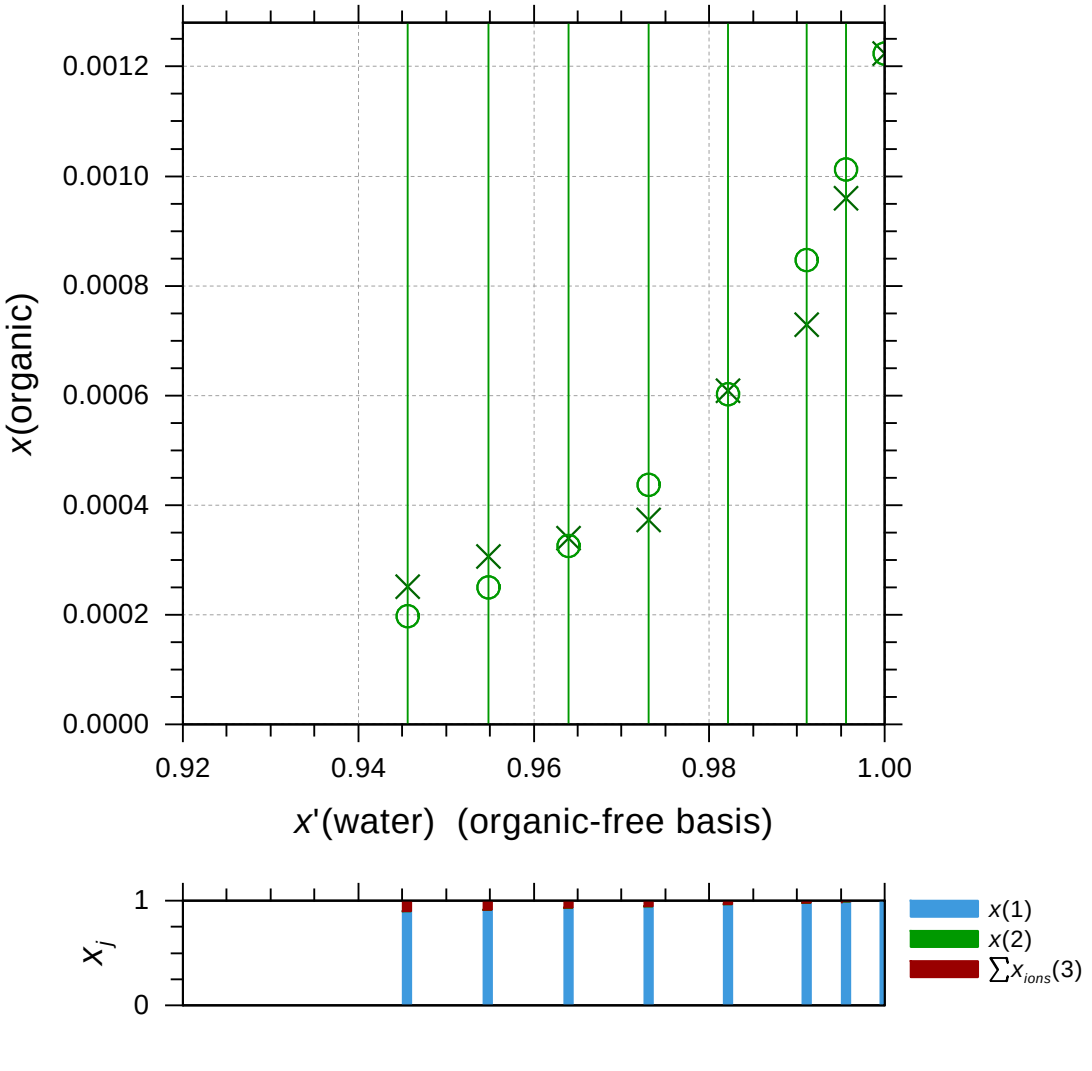
fval(0453) = 5.7967E-05

rel. contribution = 0.0000 %

Fig. S0442 (AIOMFAC_output_0456)

H_2O (1) + Gallic_acid (2) + LiCl (3)

Temperature: 298 K

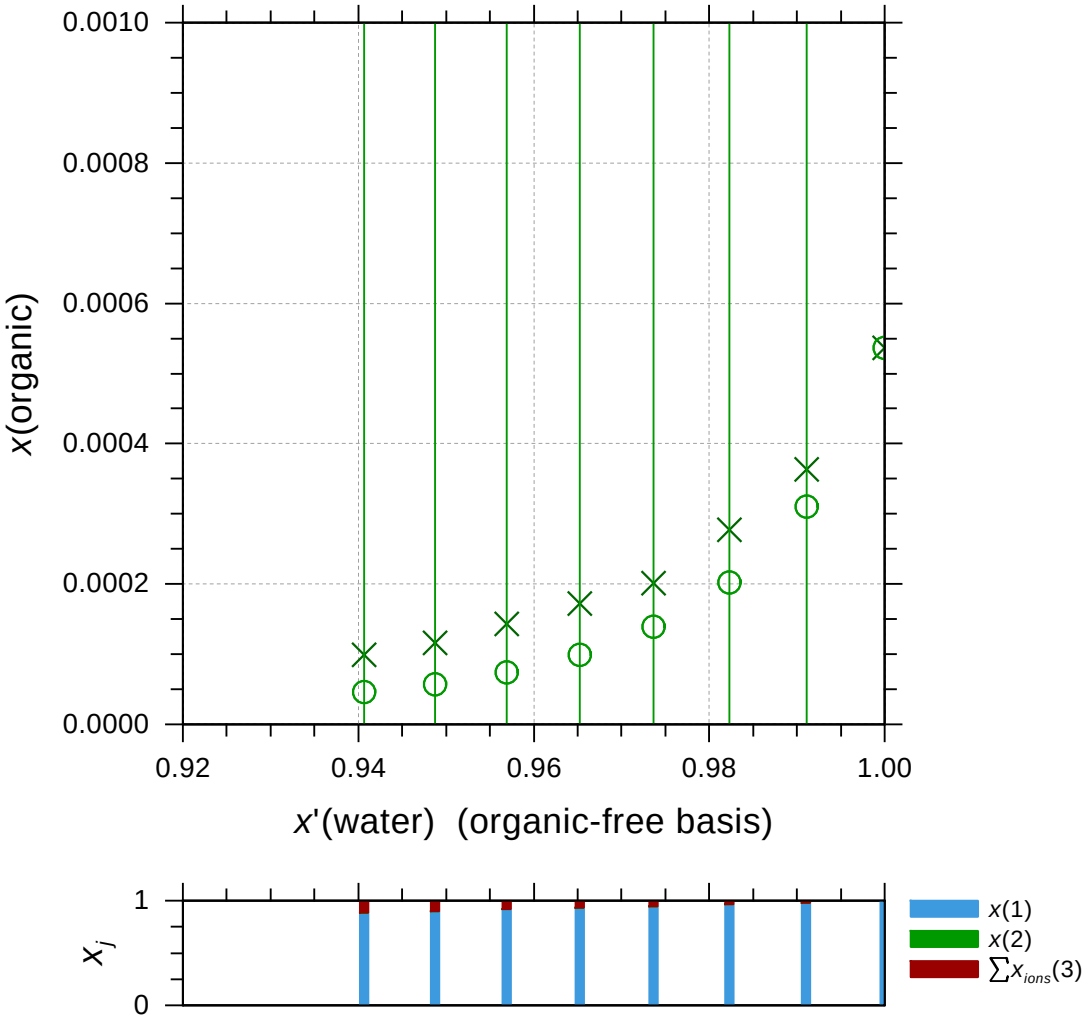


initial weighting of dataset:
w^{init}(0456) = 1.000
dataset contribution to F_{obj}:
fval(0456) = 2.4113E-04
rel. contribution = 0.0001 %

Fig. S0443 (AIOMFAC_output_0459)

H_2O (1) + Ferulic_acid (2) + LiCl (3)

Temperature: 298 K

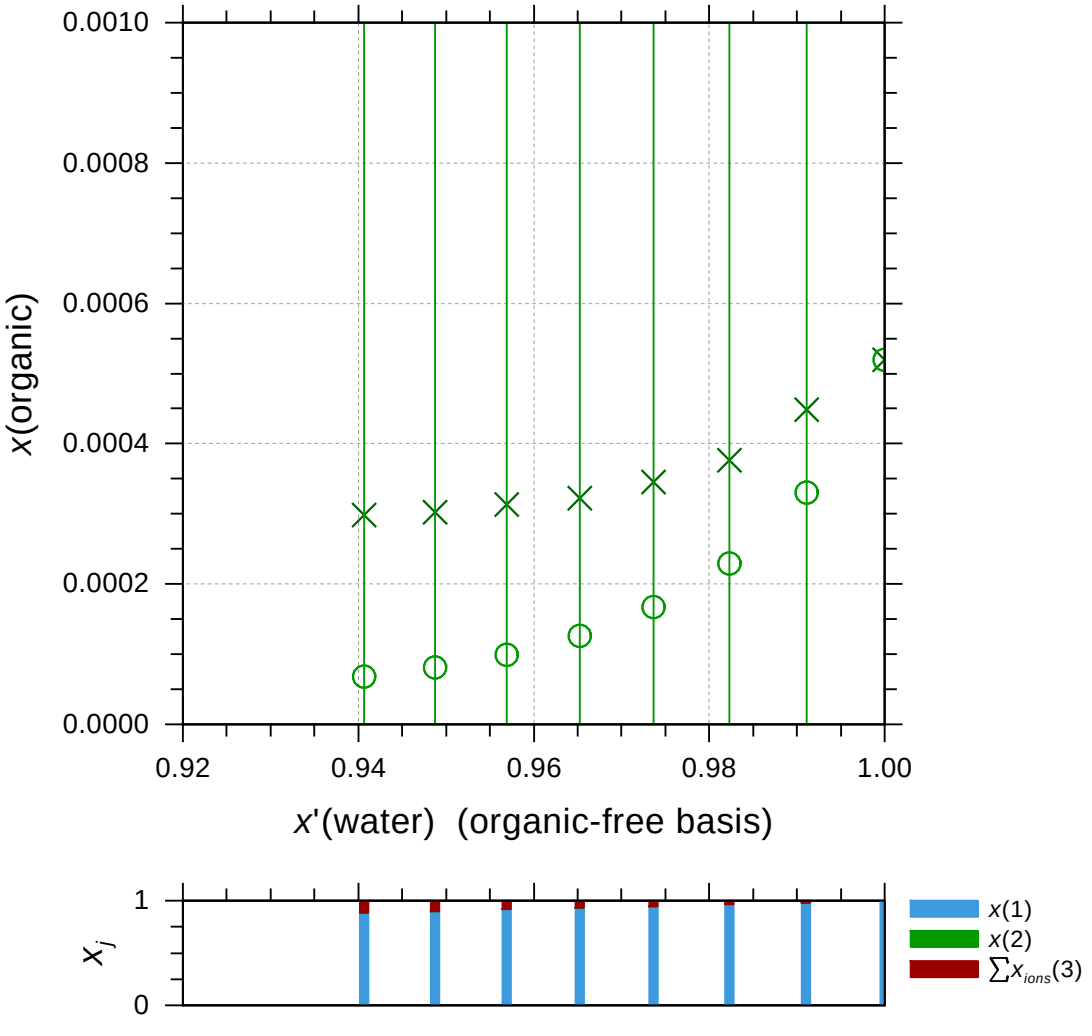


initial weighting of dataset:
w^{init}(0459) = 1.000
dataset contribution to F_{obj}:
fval(0459) = 2.7437E-04
rel. contribution = 0.0001 %

Fig. S0444 (AIOMFAC_output_0462)

H_2O (1) + Syringic_acid (2) + LiCl (3)

Temperature: 298 K

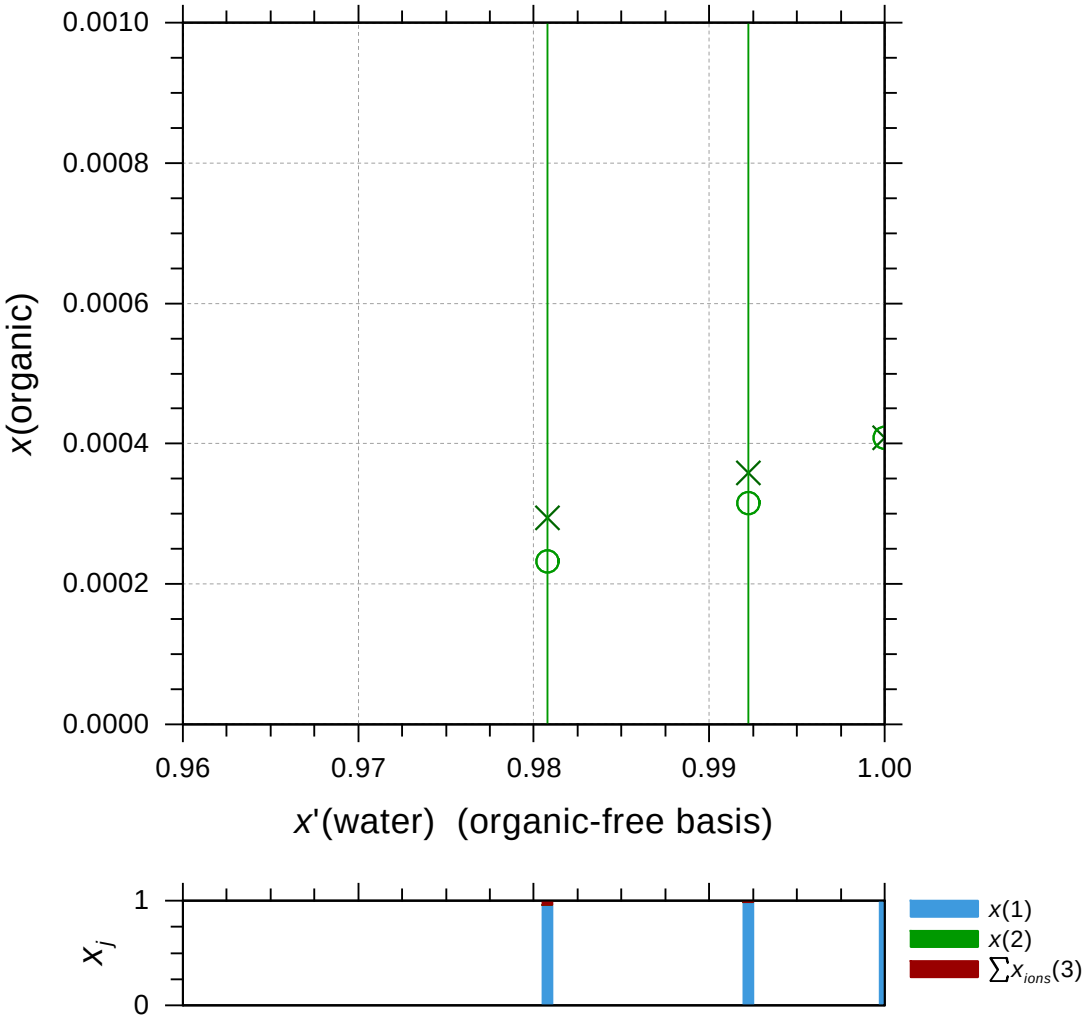


initial weighting of dataset:
w^{init}(0462) = 1.000
dataset contribution to F_{obj}:
fval(0462) = 2.3696E-03
rel. contribution = 0.0011 %

Fig. S0445 (AIOMFAC_output_0469)

H_2O (1) + Benzene (2) + LiCl (3)

Temperature: 298 K

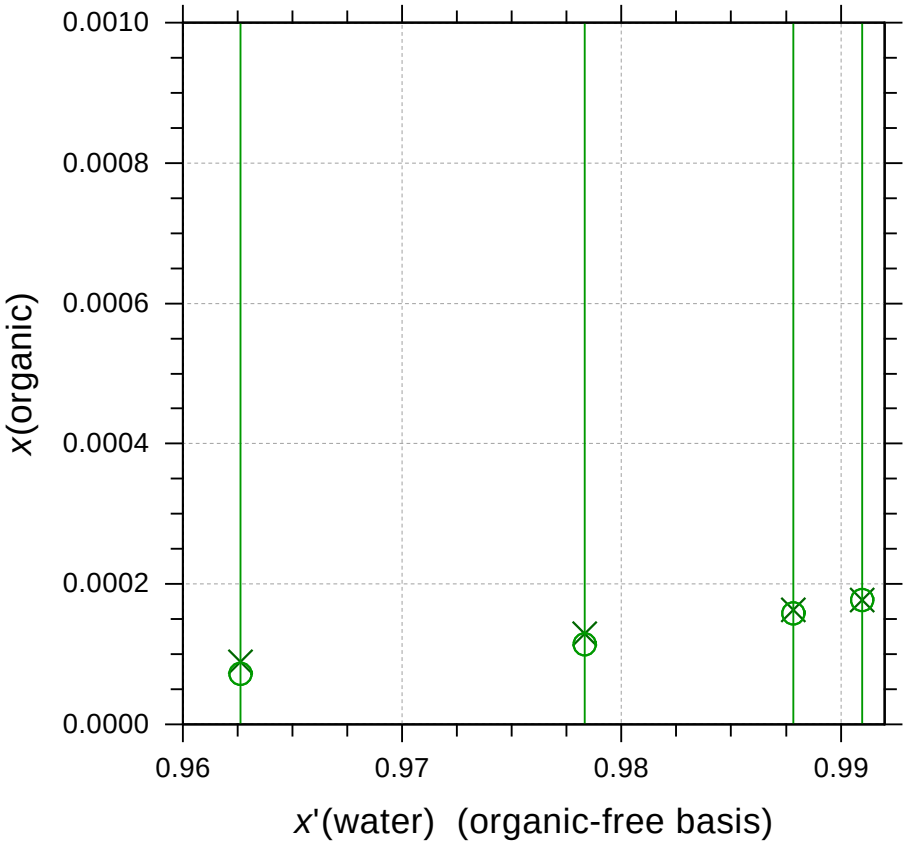


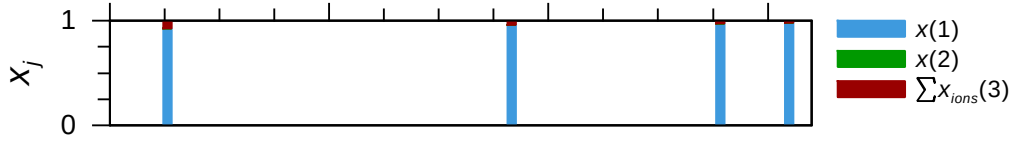
initial weighting of dataset:
$w^{init}(0469)$ = 1.000
dataset contribution to F_{obj}:
fval(0469) = 5.2905E-05
rel. contribution = 0.0000 %

Fig. S0446 (AIOMFAC_output_0476)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + LiCl (3)

Temperature: 298 K





left y-axis:

× LiCl+2-HydroxybenzoicAcid+Water_SLE_Osol

○ AIOMFAC calc. SLE composition

initial weighting of dataset:

w^{init}(0476) = 1.000

dataset contribution to F_{obj}:

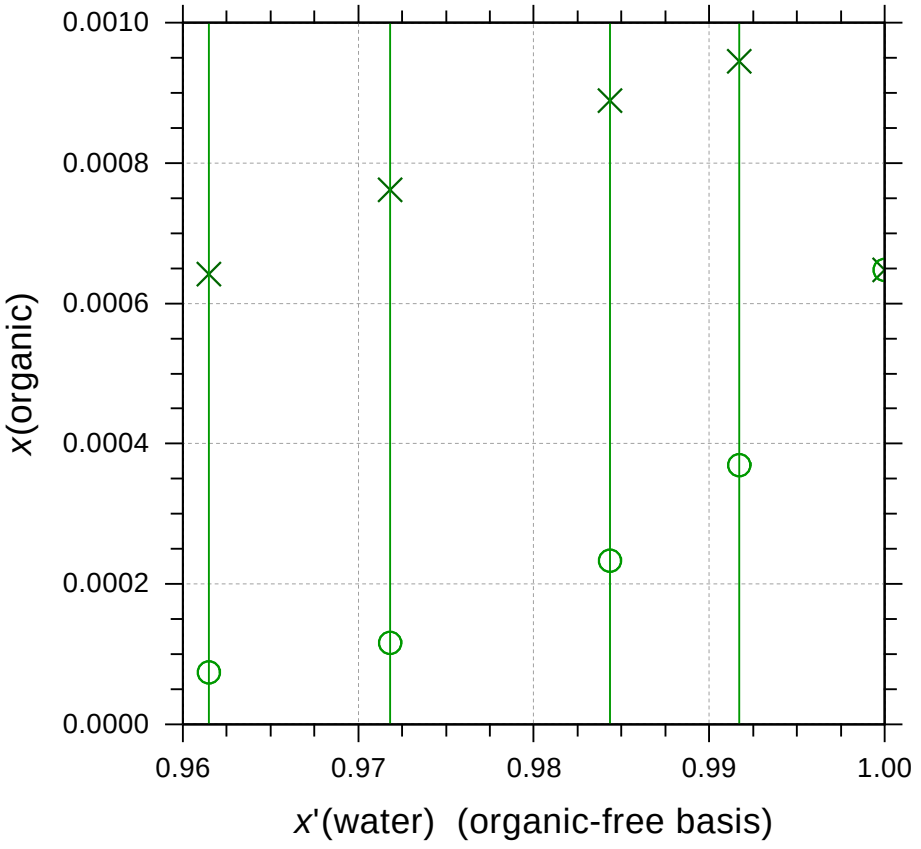
fval(0476) = 5.1837E-06

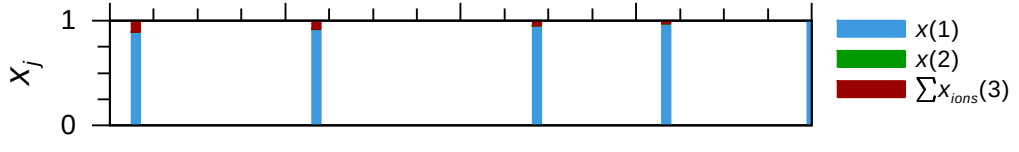
rel. contribution = 0.0000 %

Fig. S0447 (AIOMFAC_output_1002)

H_2O (1) + 2,4-Dihydroxybenzaldehyde (2) + $Mg(NO_3)_2$ (3)

Temperature: 298 K





left y-axis:

× Mg(NO3)2+2,4-Dihydroxybenzaldehyde+Water_SLE_Booth

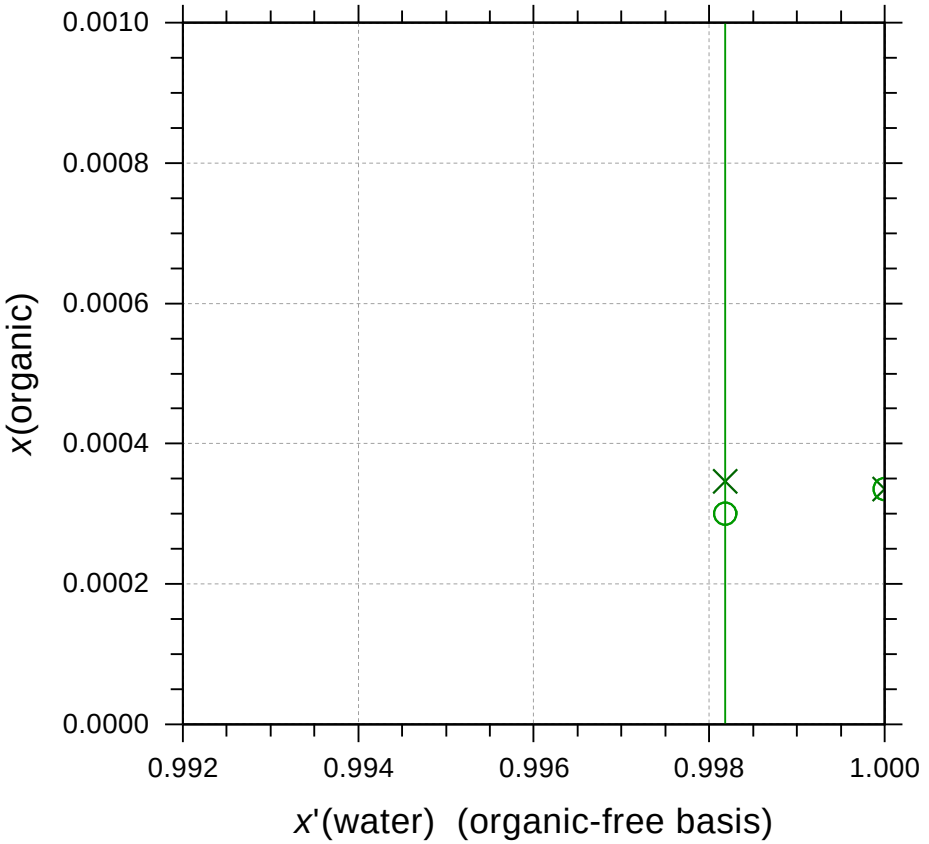
○ AIOMFAC calc. SLE composition

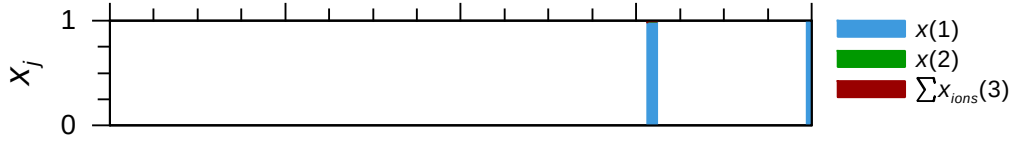
initial weighting of dataset:
w^{init}(1002) = 1.000
dataset contribution to F_{obj}:
fval(1002) = 1.2837E-02
rel. contribution = 0.0061 %

Fig. S0448 (AIOMFAC_output_0495)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + $MgSO_4$ (3)

Temperature: 298 K





left y-axis:

× MgSO4+2-HydroxybenzoicAcid+Water_SLE_Sugunan

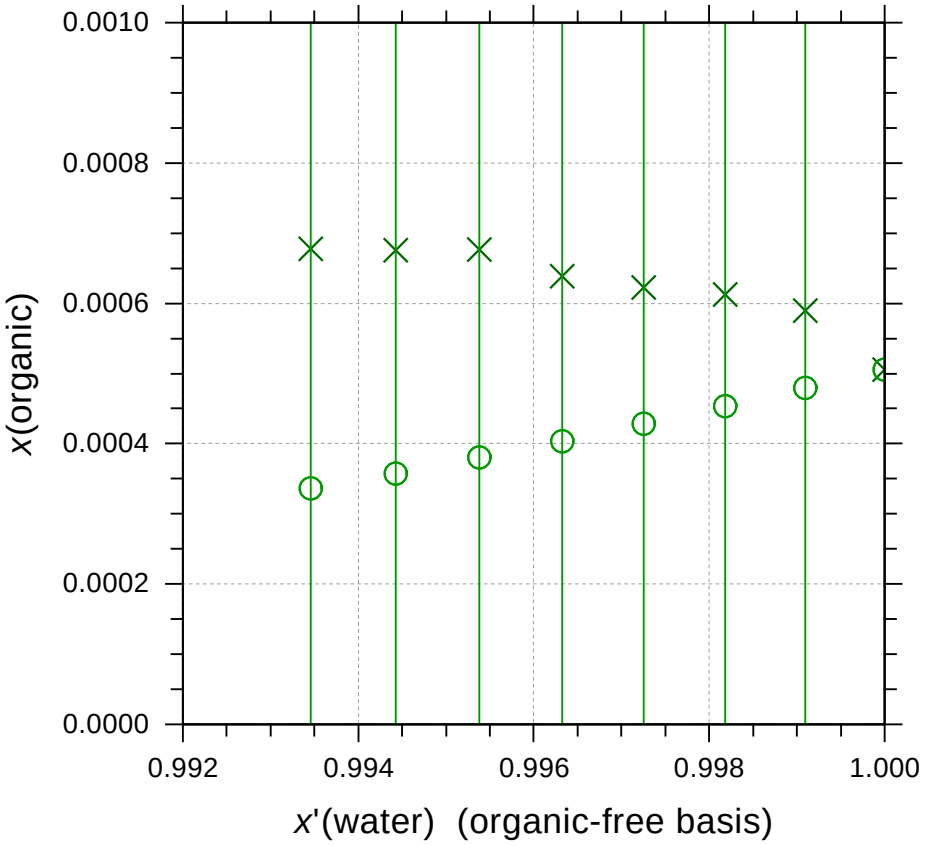
○ AIOMFAC calc. SLE composition

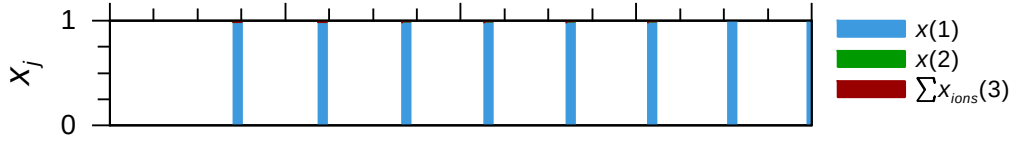
initial weighting of dataset:
w^{init}(0495) = 1.000
dataset contribution to F_{obj}:
fval(0495) = 1.9403E-05
rel. contribution = 0.0000 %

Fig. S0449 (AIOMFAC_output_0901)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + $MgSO_4$ (3)

Temperature: 308 K





left y-axis:

× MgSO4+2-HydroxybenzoicAcid+Water_SLE_308K_Sugunan

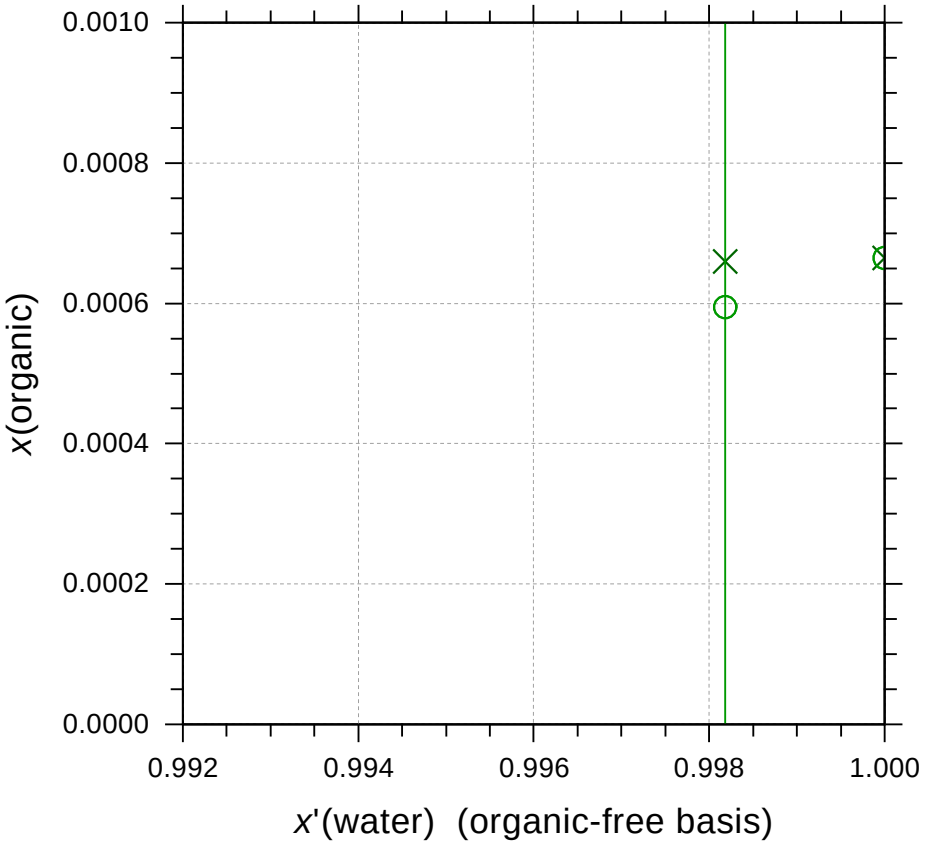
○ AIOMFAC calc. SLE composition

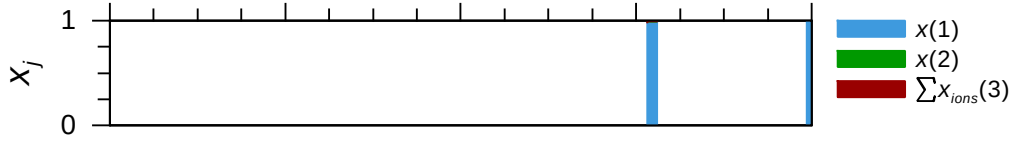
initial weighting of dataset:
w^{init}(0901) = 1.000
dataset contribution to F_{obj}:
fval(0901) = 3.8401E-03
rel. contribution = 0.0018 %

Fig. S0450 (AIOMFAC_output_0905)

H_2O (1) + 4-Hydroxybenzoic_acid (2) + $MgSO_4$ (3)

Temperature: 298 K





left y-axis:

× MgSO4+4-HydroxybenzoicAcid+Water_SLE_Sugunan

○ AIOMFAC calc. SLE composition

initial weighting of dataset:

w^{init}(0905) = 0.200

dataset contribution to F_{obj}:

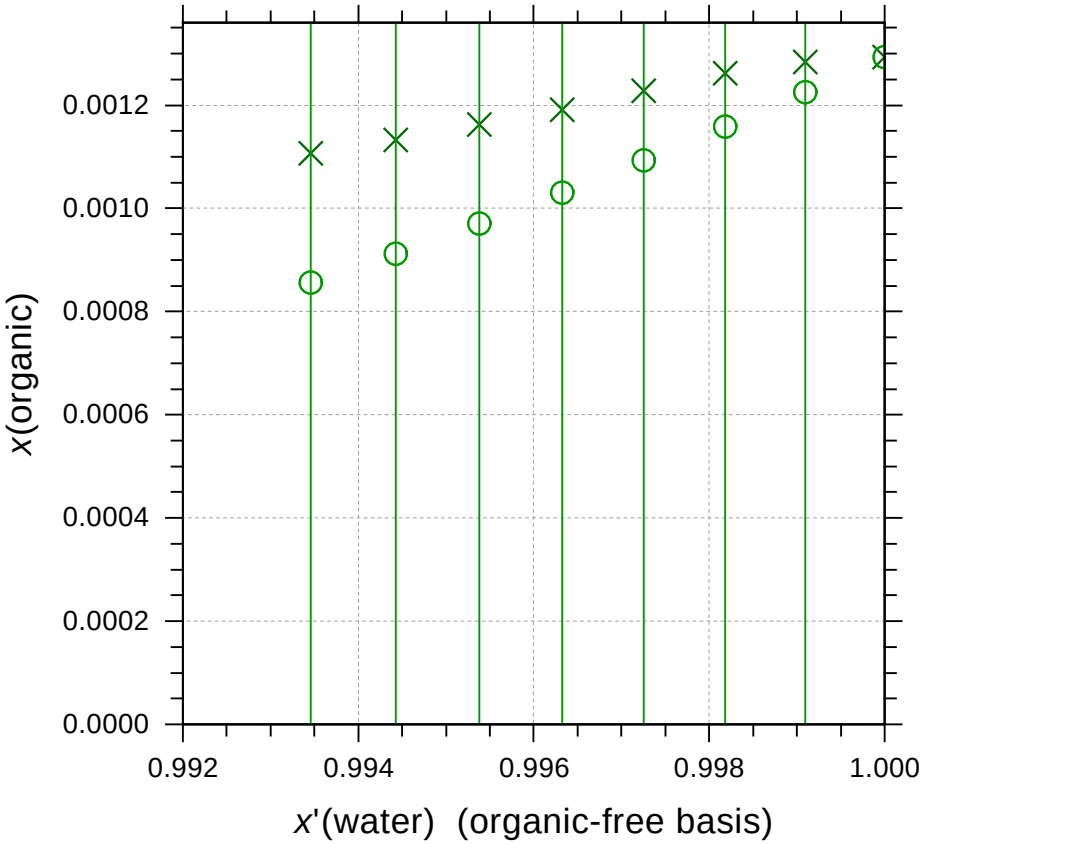
fval(0905) = 7.2877E-06

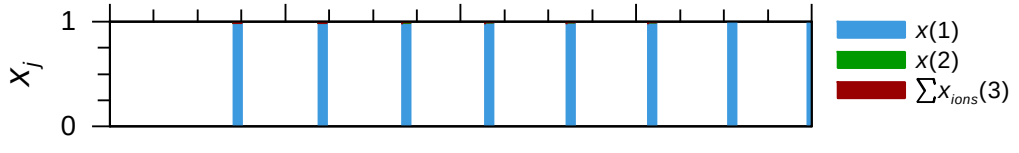
rel. contribution = 0.0000 %

Fig. S0451 (AIOMFAC_output_0909)

H_2O (1) + 4-Hydroxybenzoic_acid (2) + $MgSO_4$ (3)

Temperature: 308 K



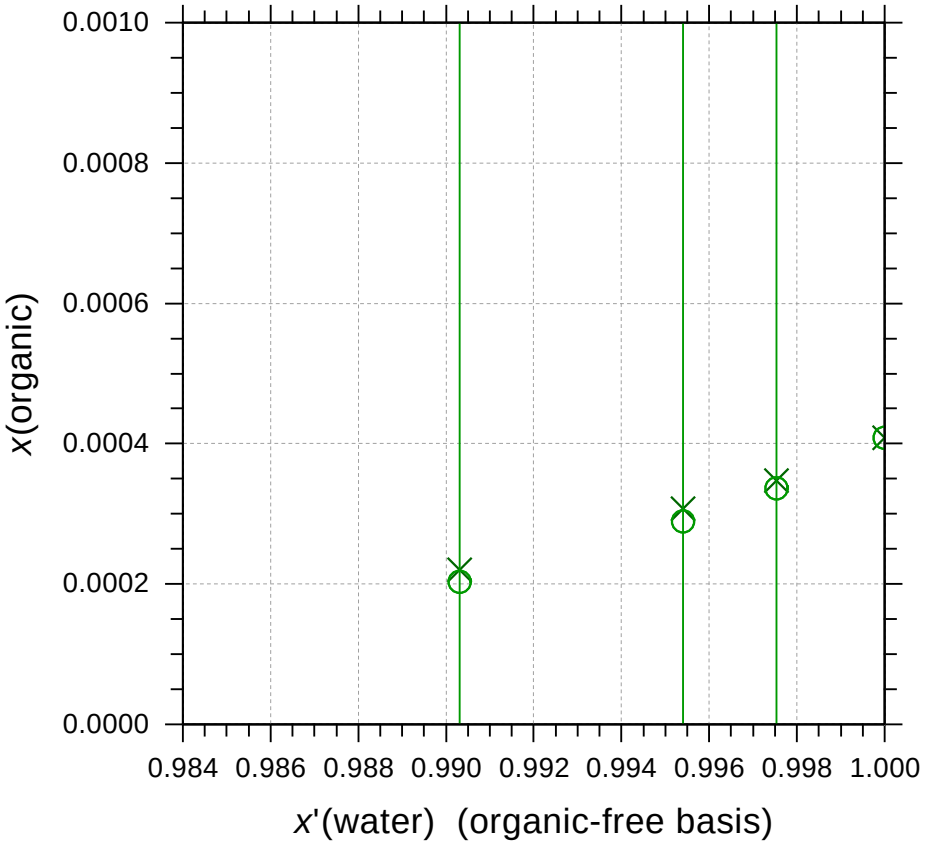


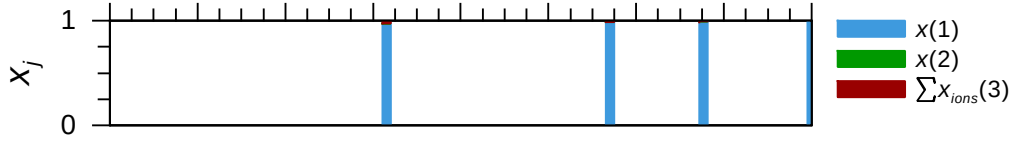
initial weighting of dataset:
$w^{init}(0909)$ = 0.200
dataset contribution to F_{obj}:
fval(0909) = 3.3169E-04
rel. contribution = 0.0002 %

Fig. S0452 (AIOMFAC_output_0463)

H_2O (1) + Benzene (2) + Na_2SO_4 (3)

Temperature: 298 K





left y-axis:

× Na2SO4+Benzene+Water_Solubility_McDevit

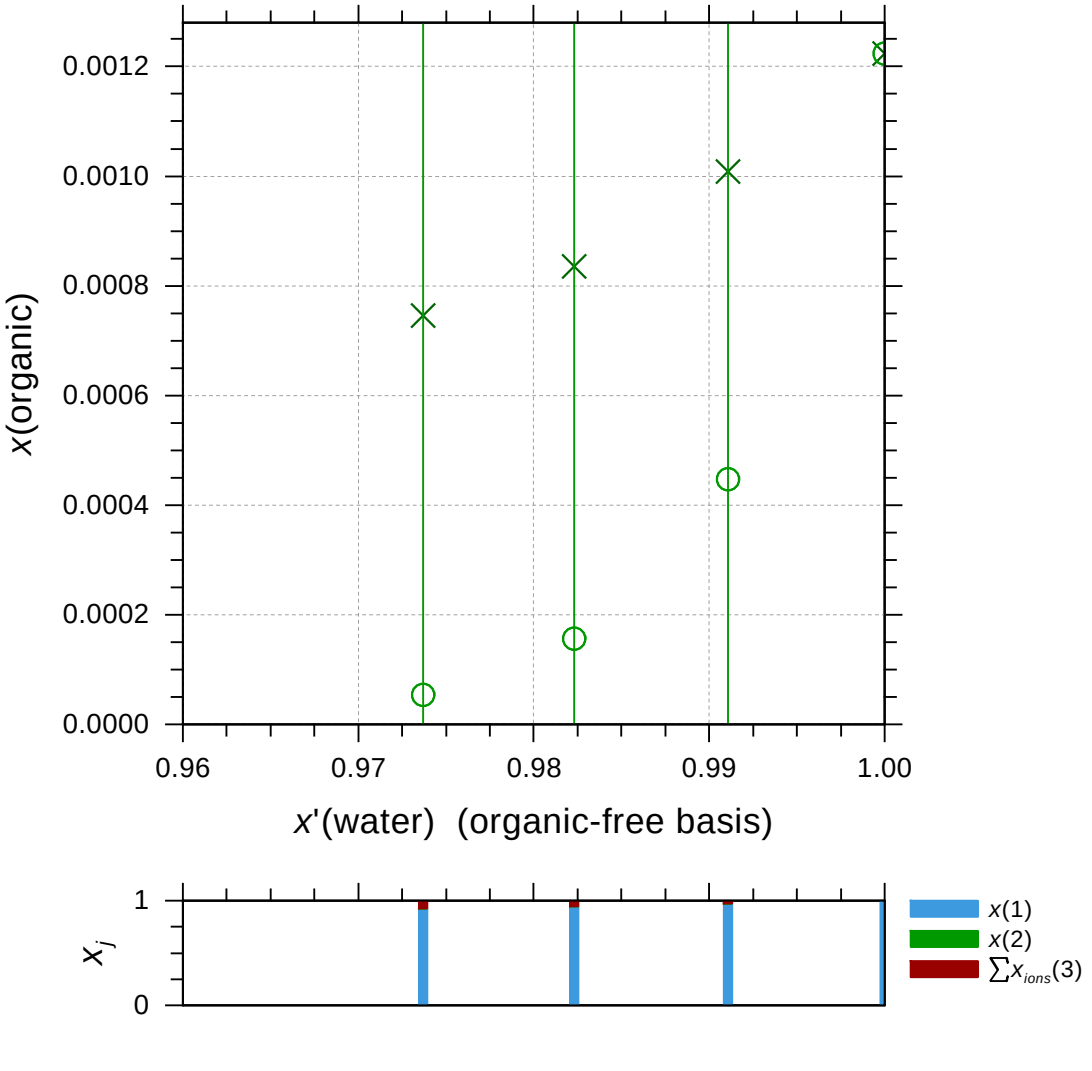
○ AIOMFAC calc. SLE composition

initial weighting of dataset:
w^{init}(0463) = 1.000
dataset contribution to F_{obj}:
fval(0463) = 6.9627E-06
rel. contribution = 0.0000 %

Fig. S0453 (AIOMFAC_output_0478)

H_2O (1) + Gallic_acid (2) + Na_2SO_4 (3)

Temperature: 298 K

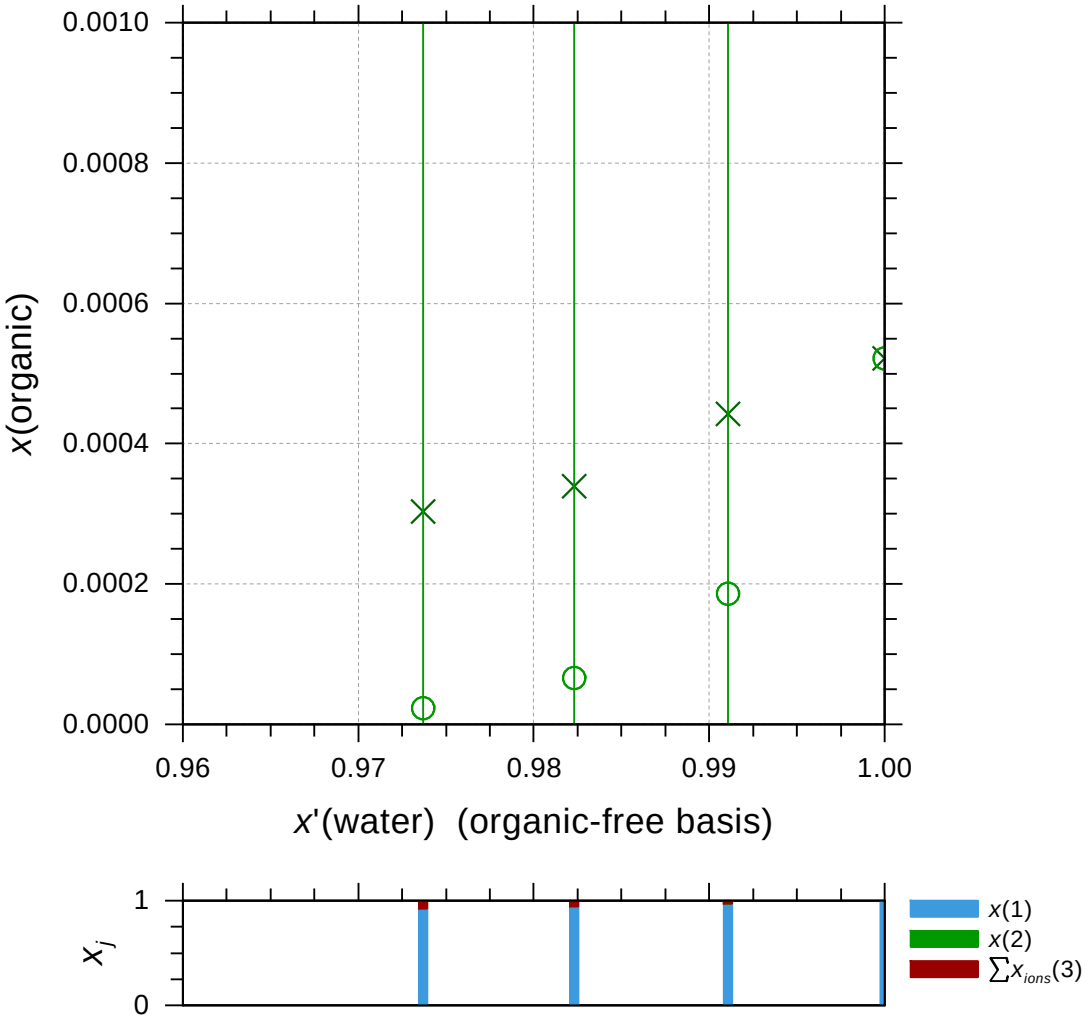


initial weighting of dataset:
w^{init}(0478) = 1.000
dataset contribution to F_{obj}:
fval(0478) = 1.0665E-02
rel. contribution = 0.0051 %

Fig. S0454 (AIOMFAC_output_0479)

H_2O (1) + Syringic_acid (2) + Na_2SO_4 (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0479)$ = 1.000

dataset contribution to F_{obj}:

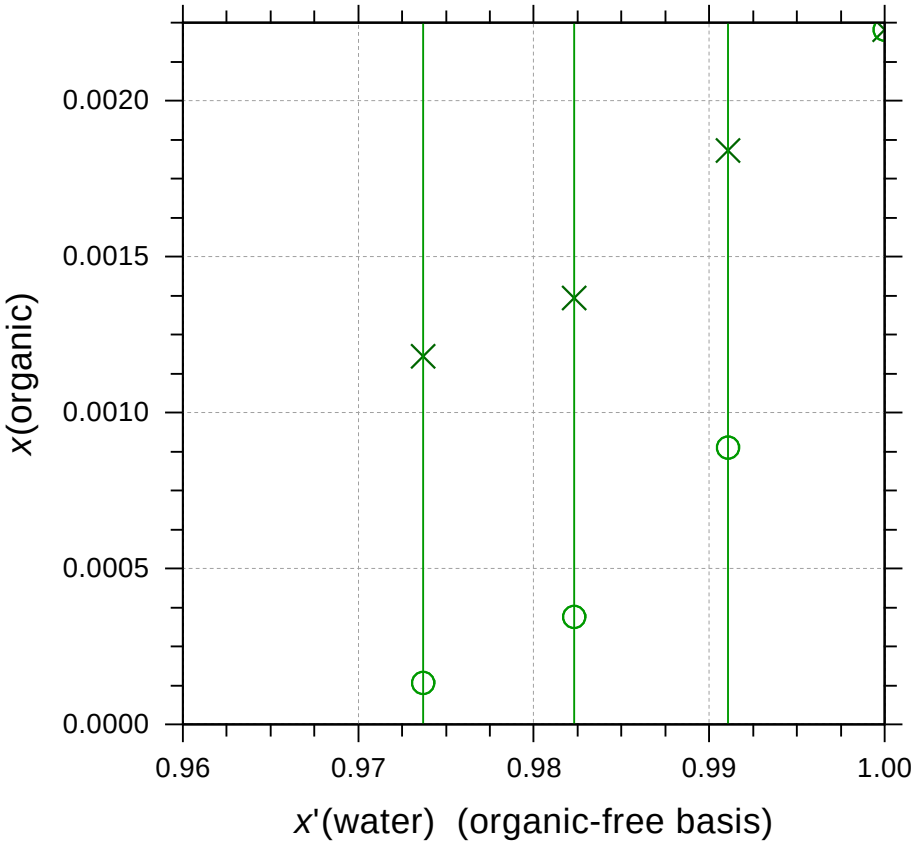
fval(0479) = 2.0396E-03

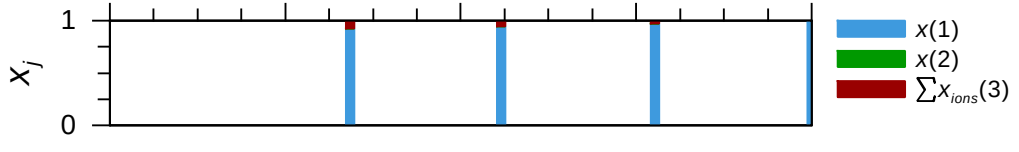
rel. contribution = 0.0010 %

Fig. S0455 (AIOMFAC_output_0480)

H_2O (1) + Protocatechuic_acid (2) + Na_2SO_4 (3)

Temperature: 298 K





left y-axis:

× Na2SO4+ProtocatechuicAcid+Water_SLE_Noubigh

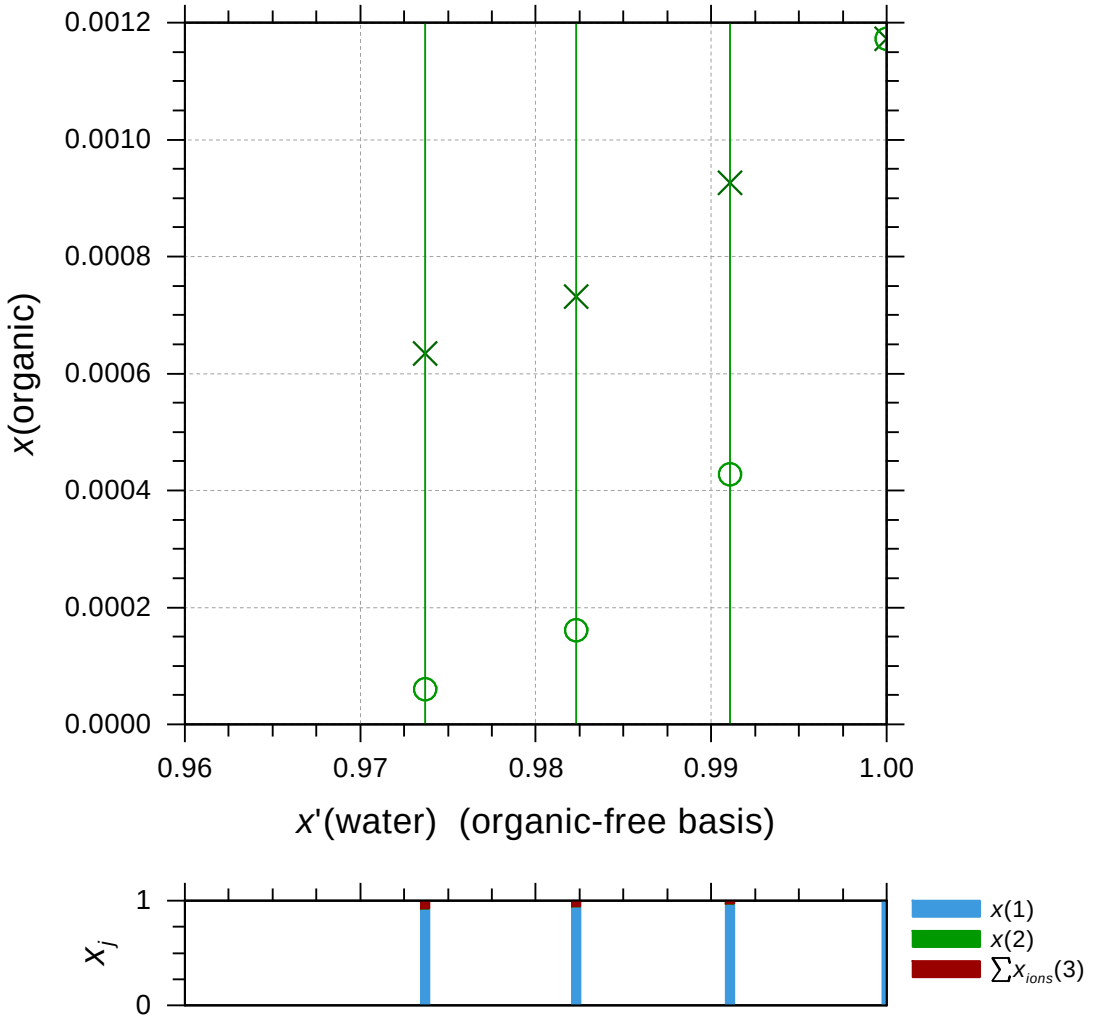
○ AIOMFAC calc. SLE composition

initial weighting of dataset:
w^{init}(0480) = 1.000
dataset contribution to F_{obj}:
fval(0480) = 2.3345E-02
rel. contribution = 0.0111 %

Fig. S0456 (AIOMFAC_output_0481)

H_2O (1) + Vanillin (2) + Na_2SO_4 (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(0481)$ = 1.000

dataset contribution to F_{obj}:

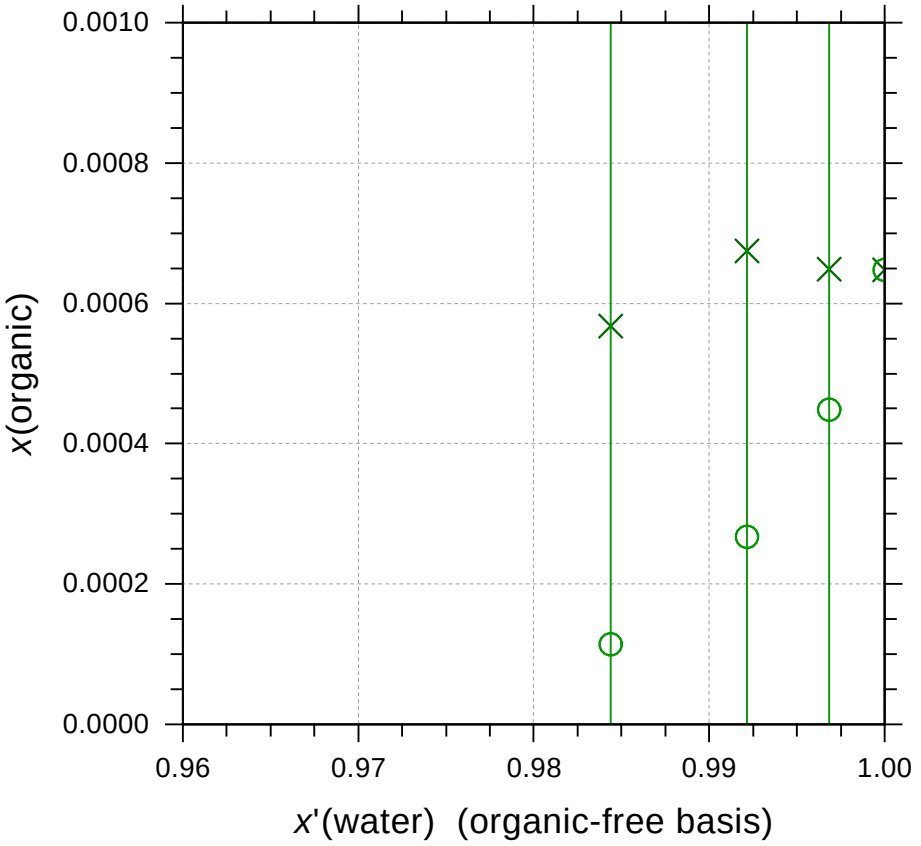
fval(0481) = 7.8236E-03

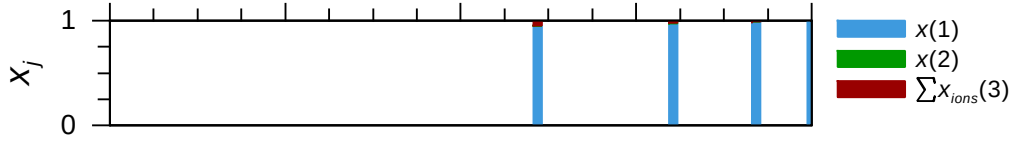
rel. contribution = 0.0037 %

Fig. S0457 (AIOMFAC_output_1005)

H_2O (1) + 2,4-Dihydroxybenzaldehyde (2) + Na_2SO_4 (3)

Temperature: 298 K





left y-axis:

× Na2SO4+2,4-Dihydroxybenzaldehyde+Water_SLE_Booth

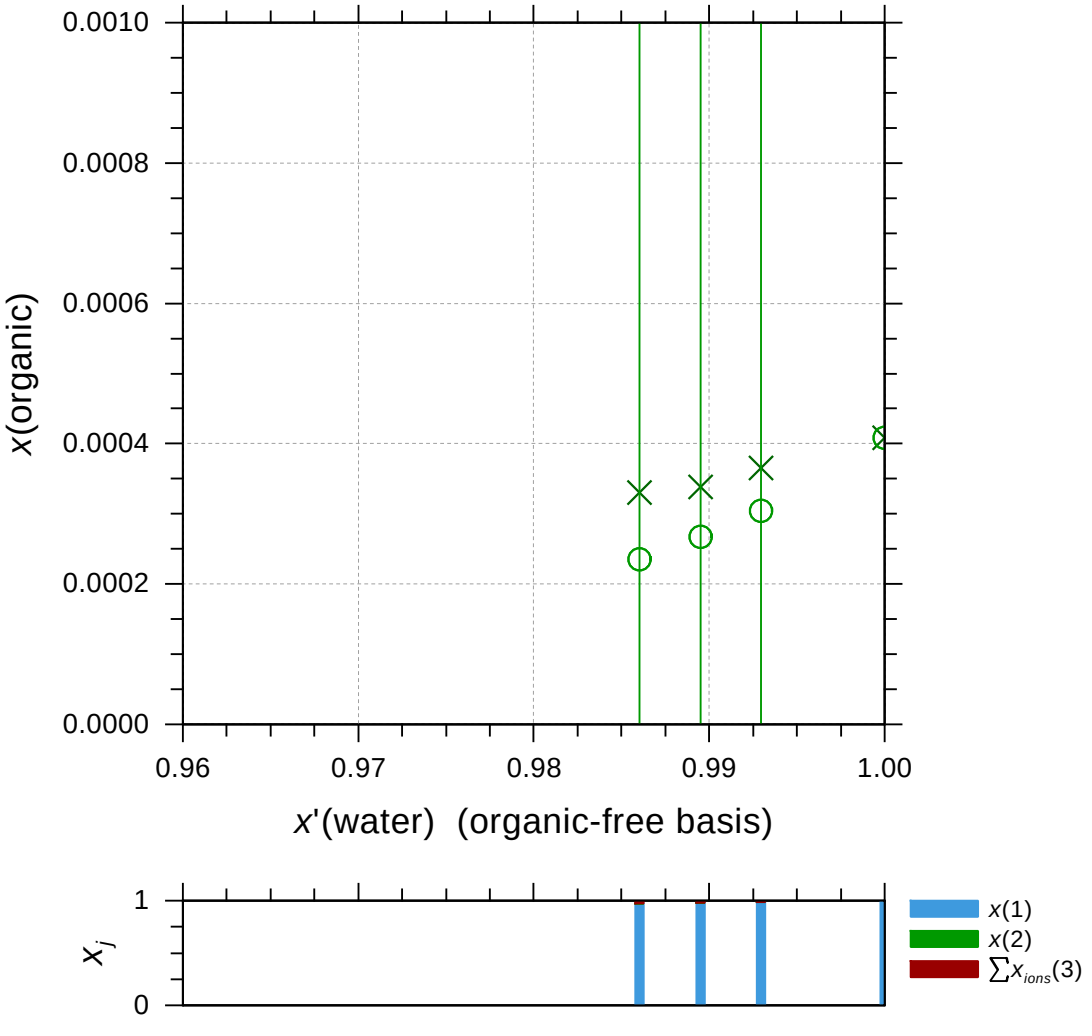
○ AIOMFAC calc. SLE composition

initial weighting of dataset:
w^{init}(1005) = 1.000
dataset contribution to F_{obj}:
fval(1005) = 3.6497E-03
rel. contribution = 0.0017 %

Fig. S0458 (AIOMFAC_output_0465)

H_2O (1) + Benzene (2) + NaBr (3)

Temperature: 298 K

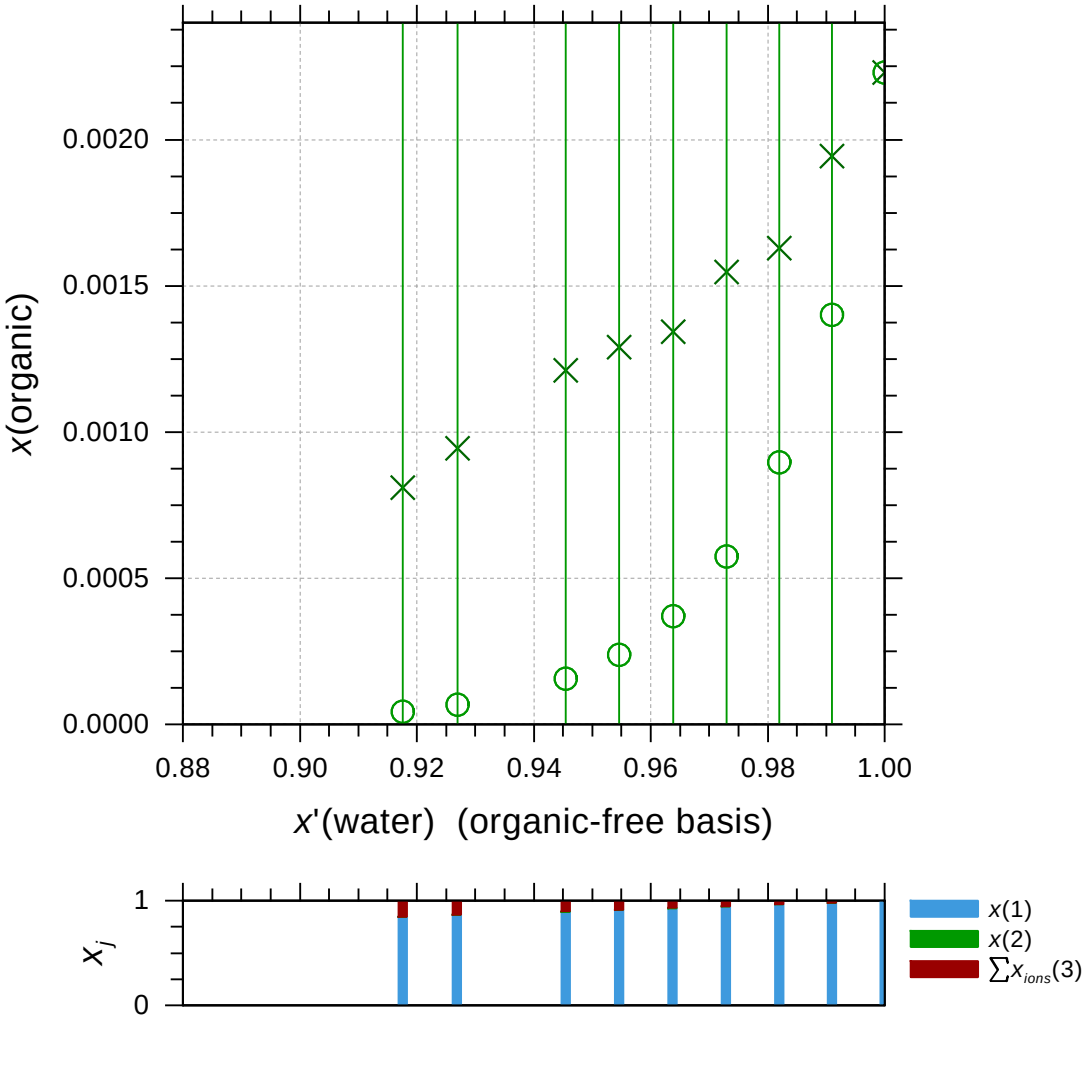


initial weighting of dataset:
$w^{init}(0465)$ = 1.000
dataset contribution to F_{obj}:
fval(0465) = 1.6746E-04
rel. contribution = 0.0001 %

Fig. S0459 (AIOMFAC_output_0446)

H_2O (1) + Protocatechuic_acid (2) + NaCl (3)

Temperature: 298 K

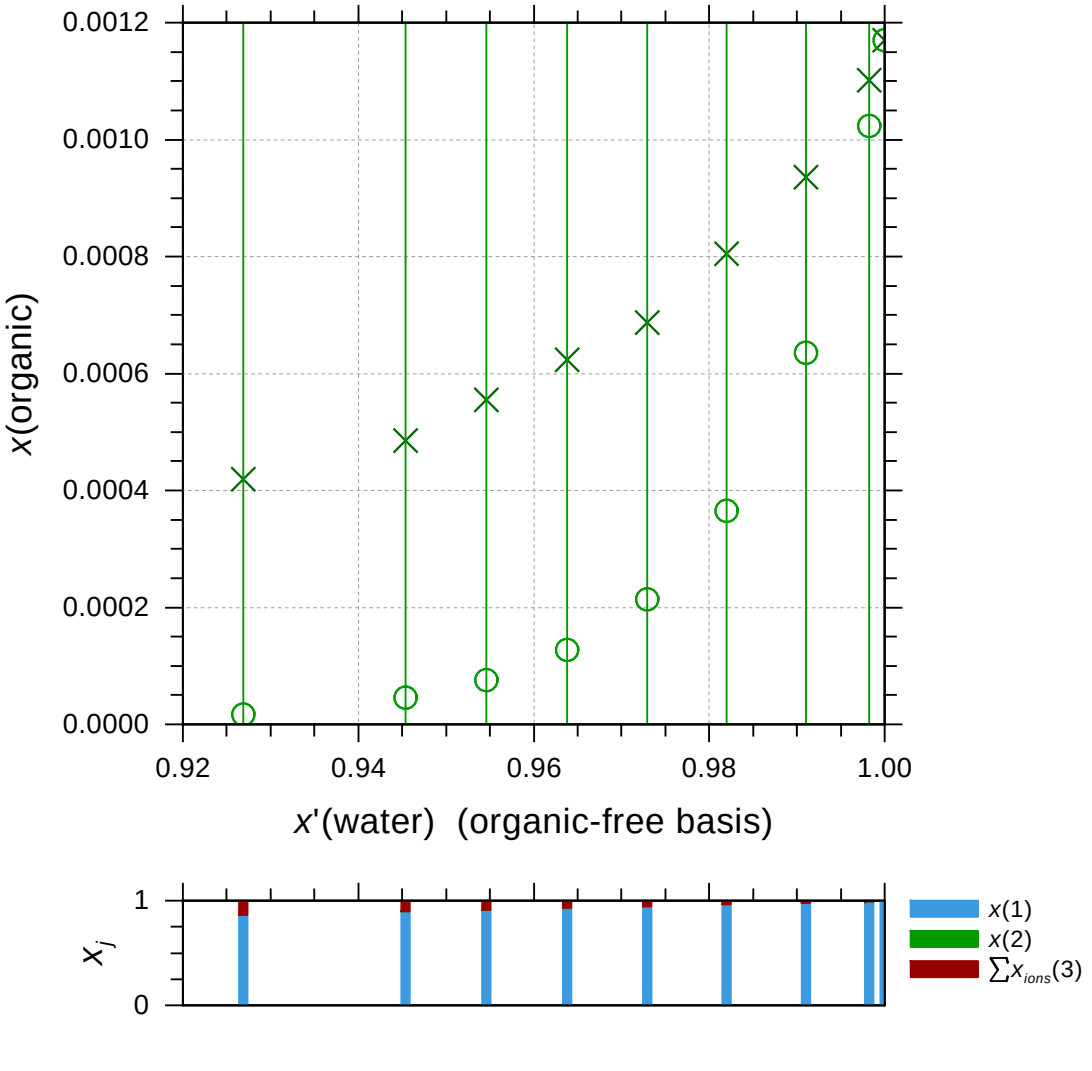


initial weighting of dataset:
w^{init}(0446) = 1.000
dataset contribution to F_{obj}:
fval(0446) = 4.9470E-02
rel. contribution = 0.0235 %

Fig. S0460 (AIOMFAC_output_0449)

H_2O (1) + Vanillin (2) + NaCl (3)

Temperature: 298 K

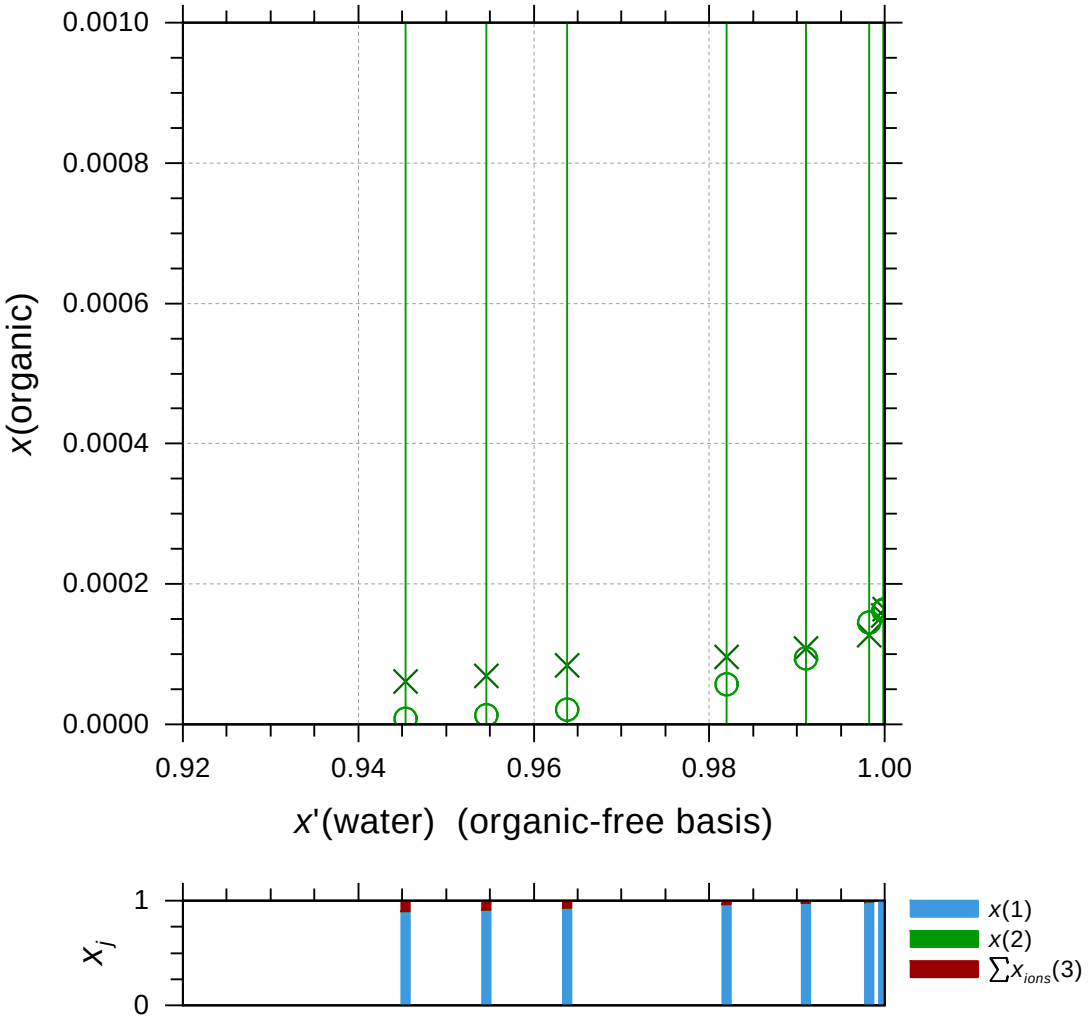


initial weighting of dataset:
w^{init}(0449) = 1.000
dataset contribution to F_{obj}:
fval(0449) = 1.1919E-02
rel. contribution = 0.0057 %

Fig. S0461 (AIOMFAC_output_0452)

H_2O (1) + Vanillic_acid (2) + NaCl (3)

Temperature: 298 K

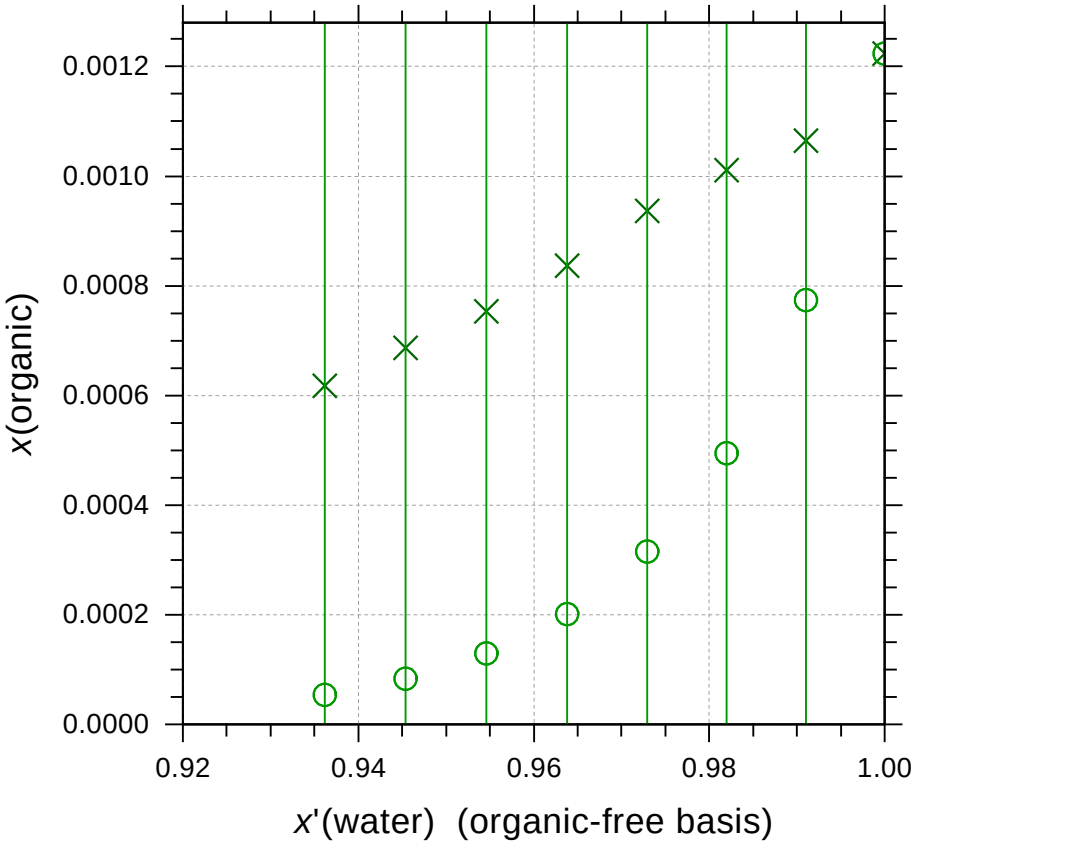


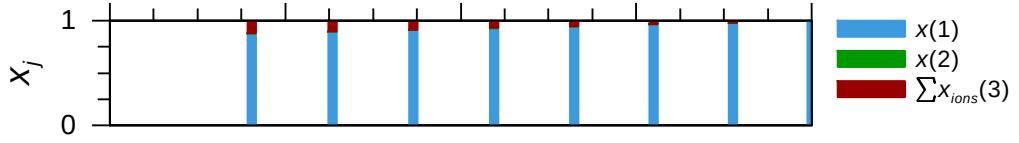
initial weighting of dataset:
w^{init}(0452) = 1.000
dataset contribution to F_{obj}:
fval(0452) = 1.1741E-04
rel. contribution = 0.0001 %

Fig. S0462 (AIOMFAC_output_0455)

H_2O (1) + Gallic_acid (2) + NaCl (3)

Temperature: 298 K



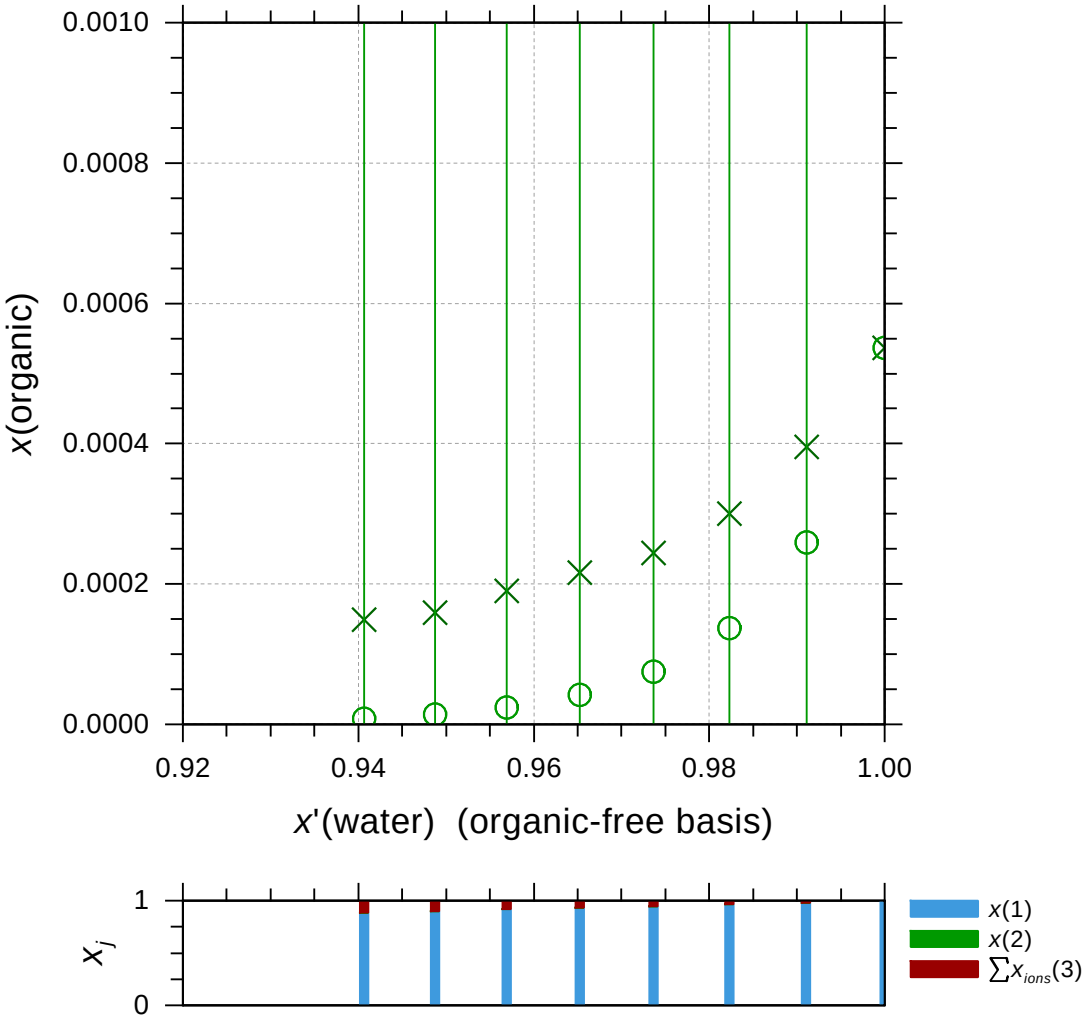


initial weighting of dataset:
w^{init}(0455) = 1.000
dataset contribution to F_{obj}:
fval(0455) = 1.8924E-02
rel. contribution = 0.0090 %

Fig. S0463 (AIOMFAC_output_0458)

H_2O (1) + Ferulic_acid (2) + NaCl (3)

Temperature: 298 K

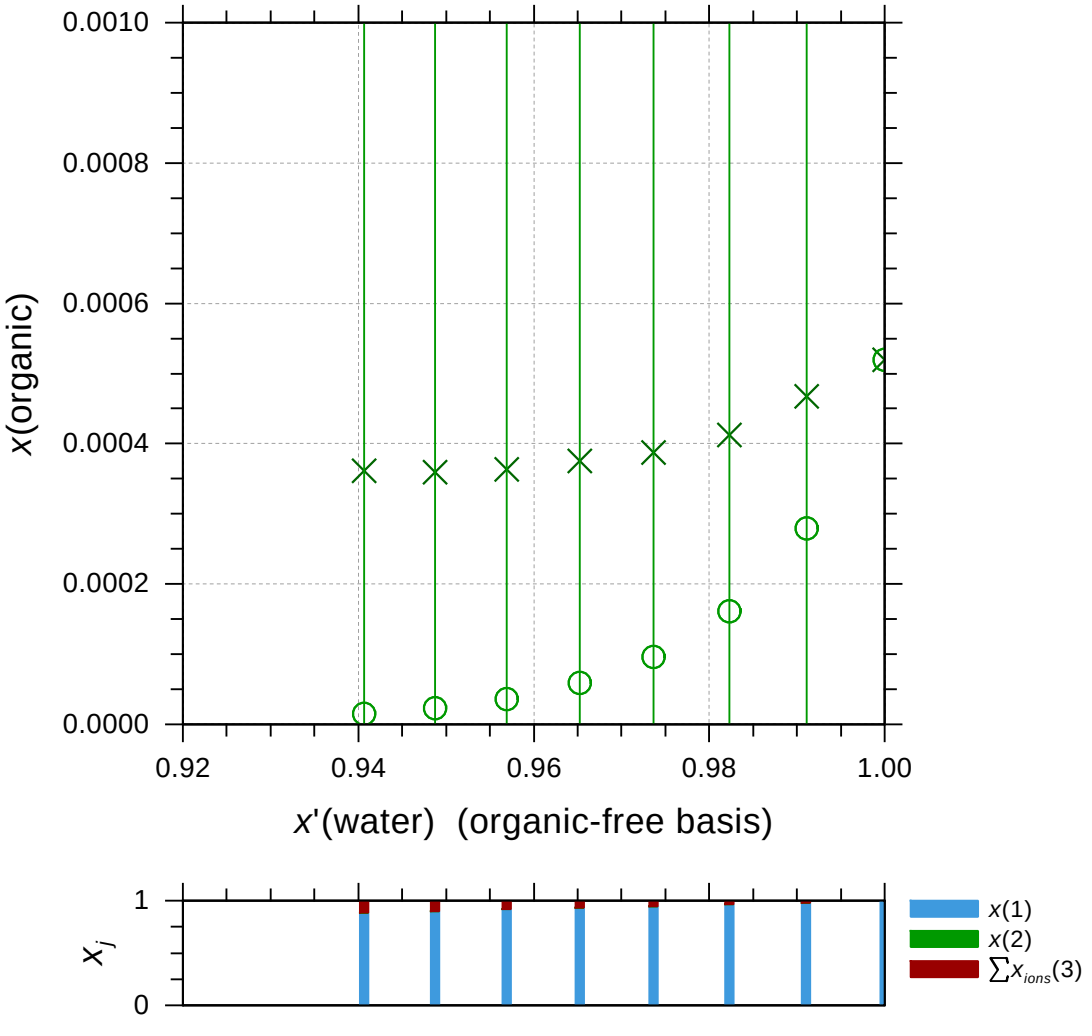


initial weighting of dataset:
w^{init}(0458) = 1.000
dataset contribution to F_{obj}:
fval(0458) = 1.6420E-03
rel. contribution = 0.0008 %

Fig. S0464 (AIOMFAC_output_0461)

H_2O (1) + Syringic_acid (2) + NaCl (3)

Temperature: 298 K

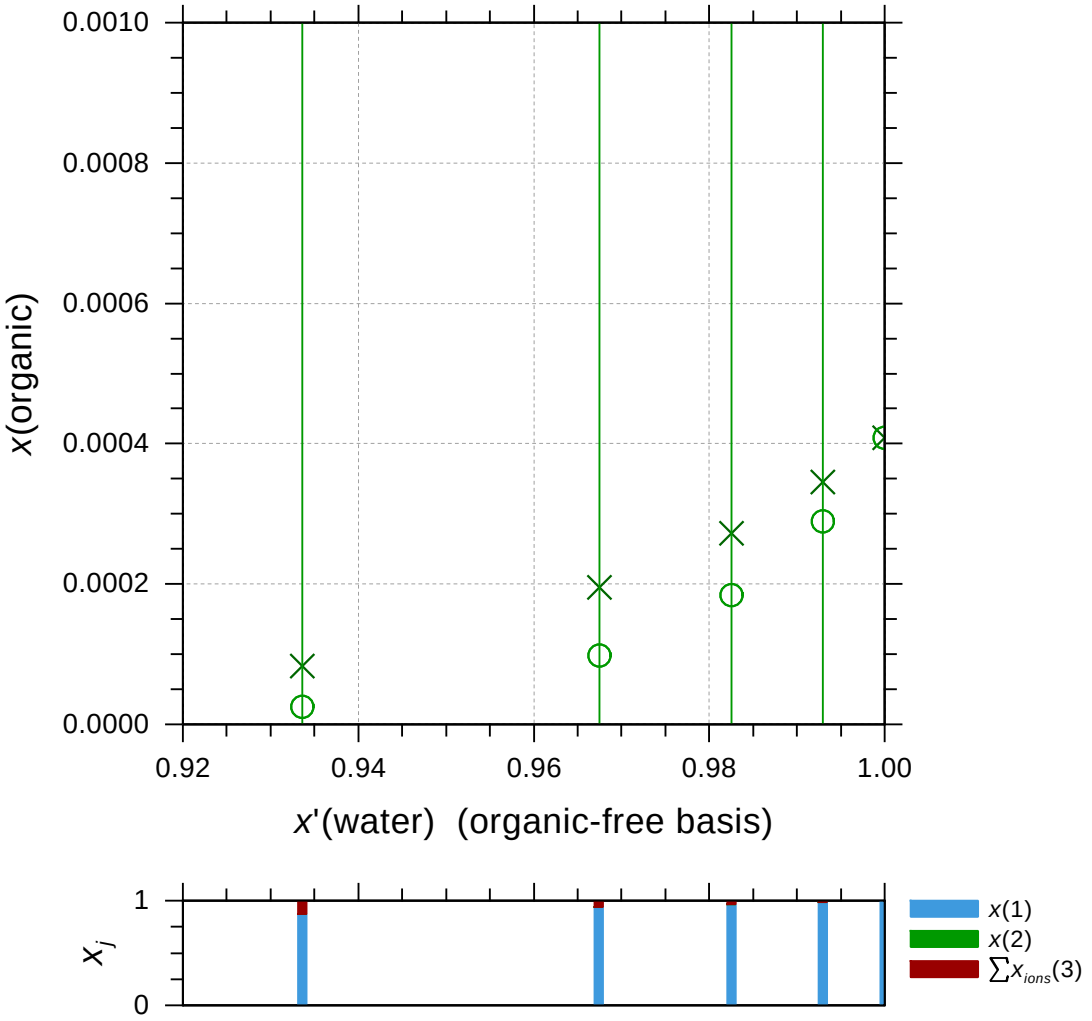


initial weighting of dataset:
w^{init}(0461) = 1.000
dataset contribution to F_{obj}:
fval(0461) = 5.7823E-03
rel. contribution = 0.0027 %

Fig. S0465 (AIOMFAC_output_0464)

H_2O (1) + Benzene (2) + NaCl (3)

Temperature: 298 K

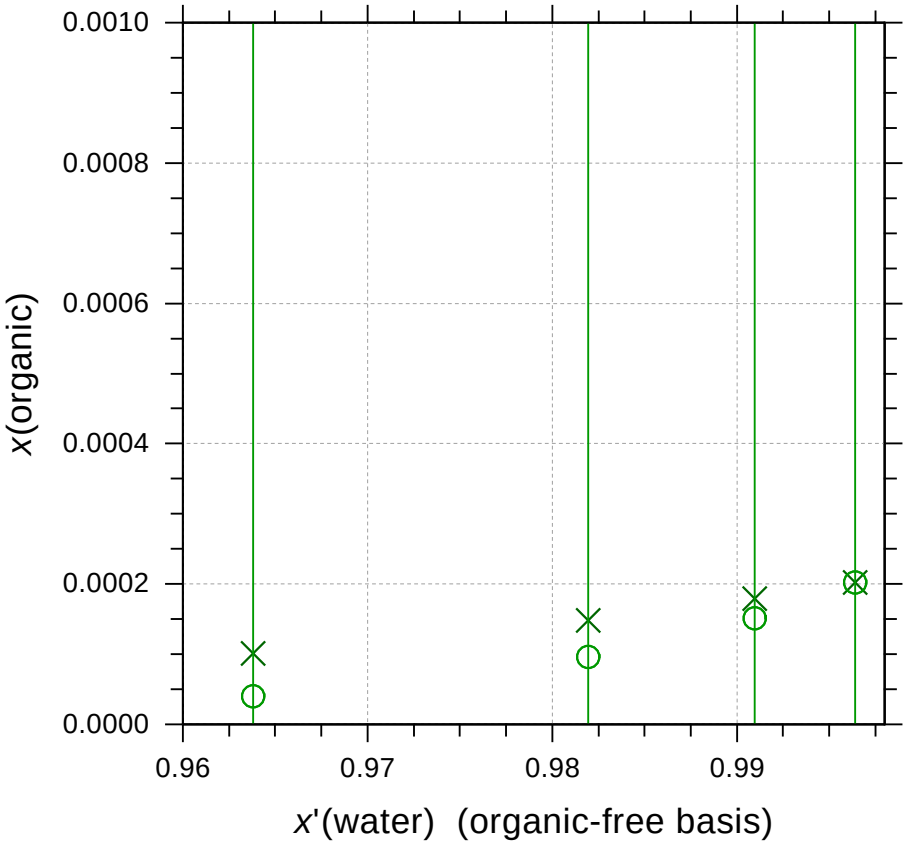


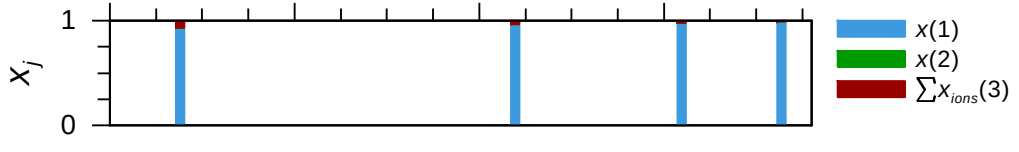
initial weighting of dataset:
w^{init}(0464) = 1.000
dataset contribution to F_{obj}:
fval(0464) = 2.2628E-04
rel. contribution = 0.0001 %

Fig. S0466 (AIOMFAC_output_0475)

H_2O (1) + 2-Hydroxybenzoic_acid (2) + NaCl (3)

Temperature: 298 K



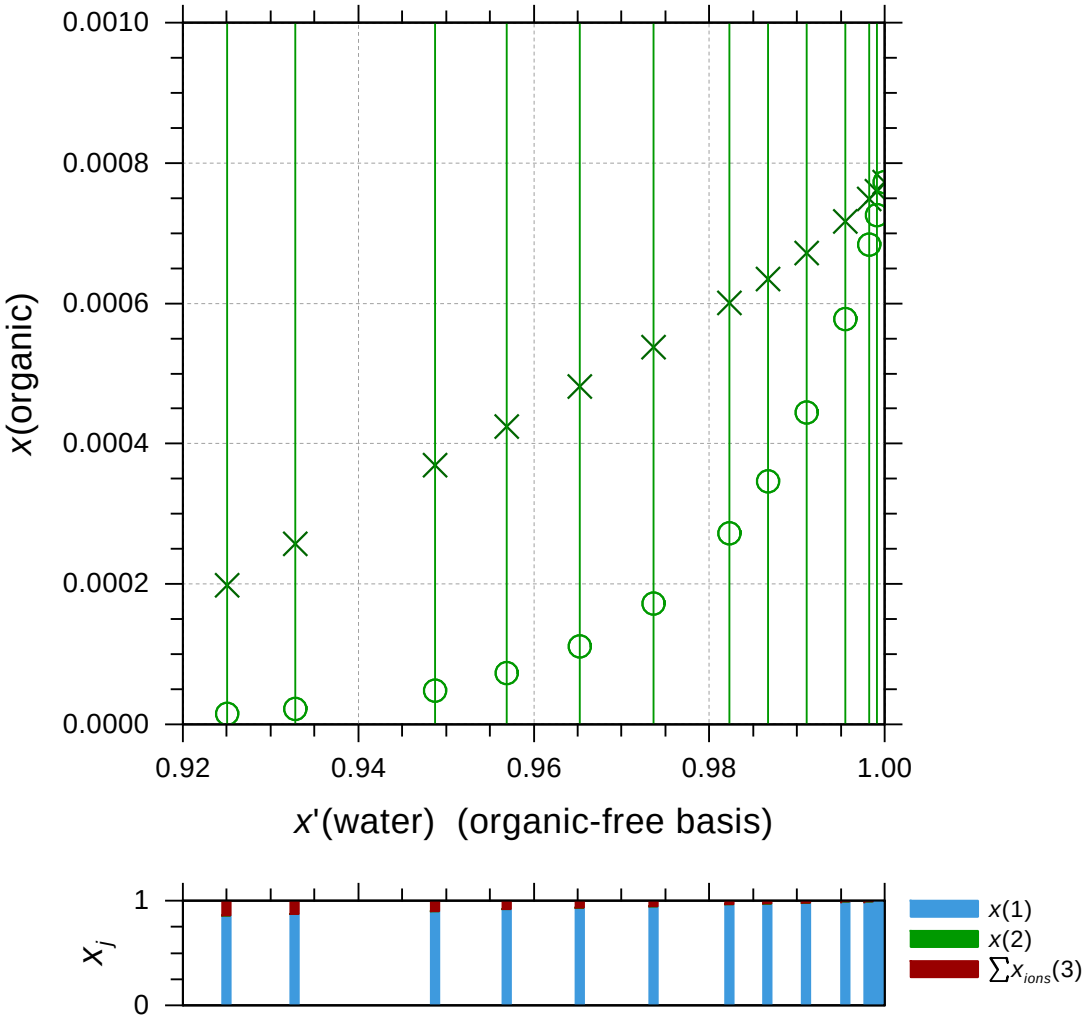


initial weighting of dataset:
w^{init}(0475) = 1.000
dataset contribution to F_{obj}:
fval(0475) = 7.0444E-05
rel. contribution = 0.0000 %

Fig. S0467 (AIOMFAC_output_0482)

H_2O (1) + Phthalic_acid (2) + NaCl (3)

Temperature: 298 K

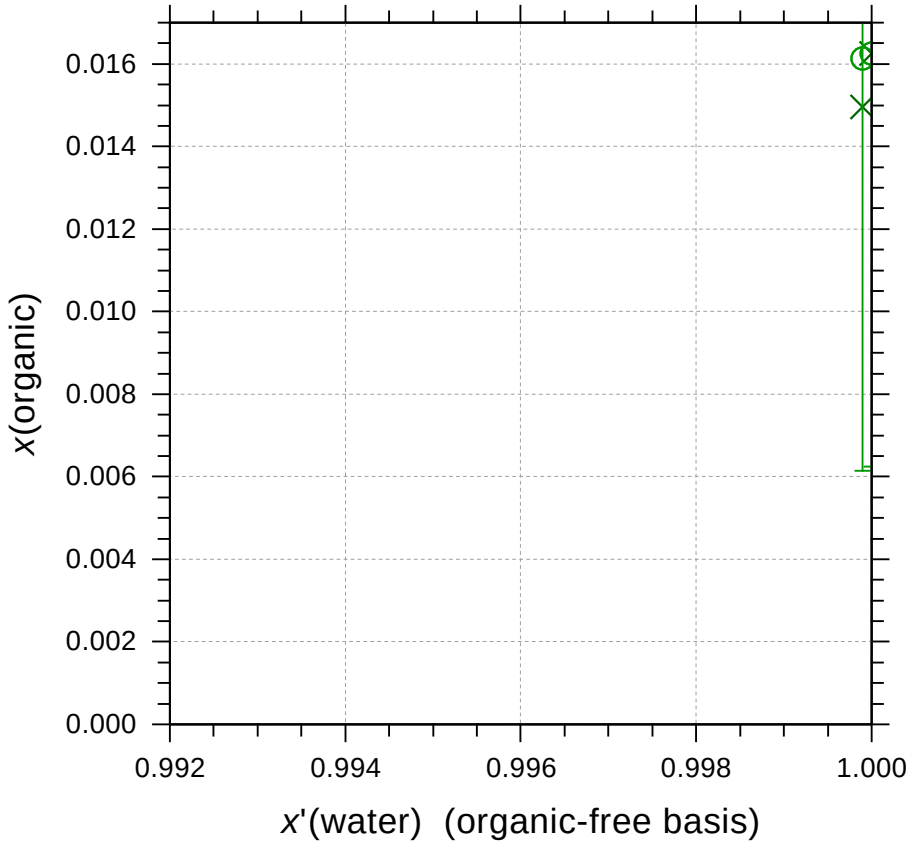


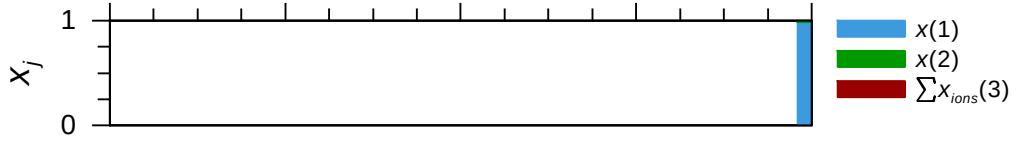
initial weighting of dataset:
$w^{init}(0482)$ = 1.000
dataset contribution to F_{obj}:
fval(0482) = 5.9707E-03
rel. contribution = 0.0028 %

Fig. S0468 (AIOMFAC_output_0483)

H_2O (1) + Phenol (2) + NaCl (3)

Temperature: 300 K





left y-axis:

× NaCl+Phenol+Water_Solubility_Jaoui

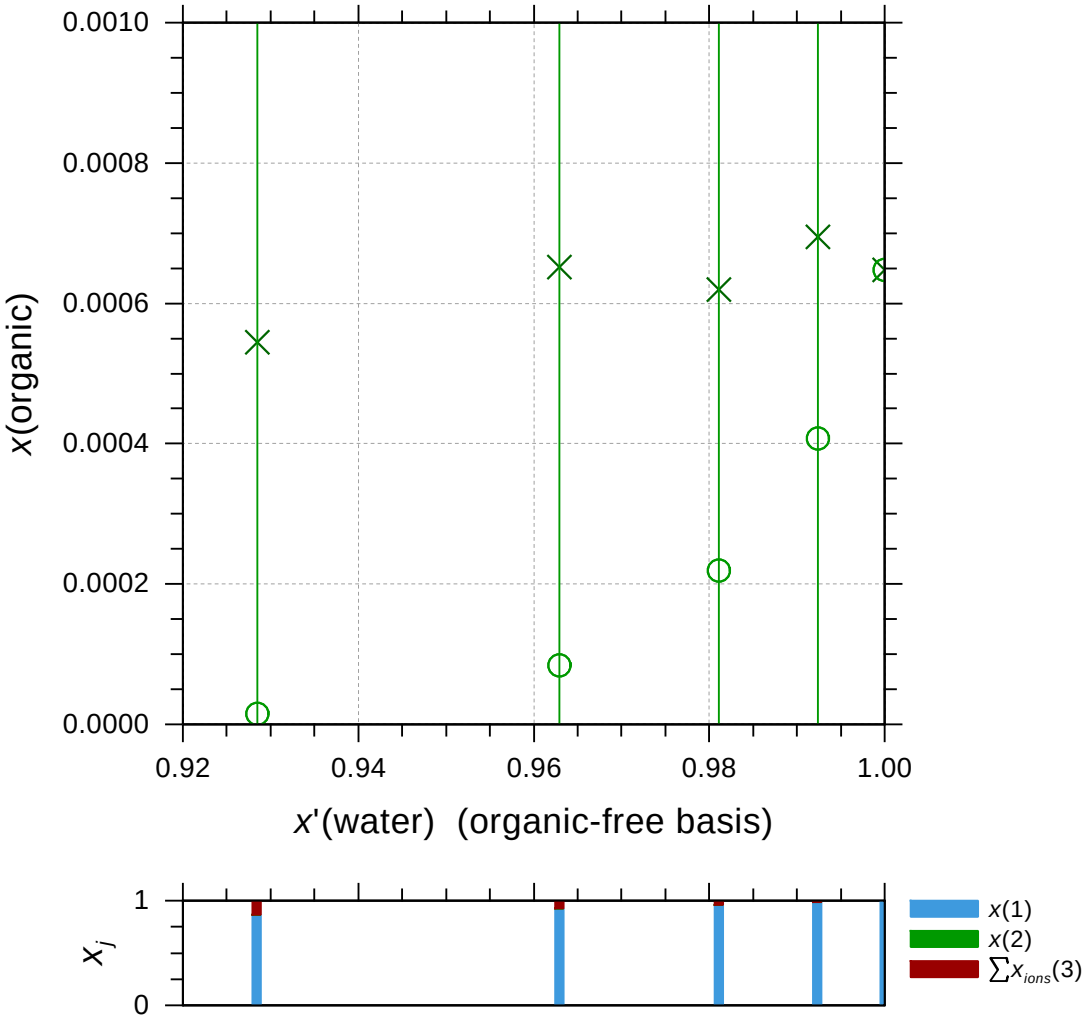
○ AIOMFAC calc. SLE composition

initial weighting of dataset:
w^{init}(0483) = 1.000
dataset contribution to F_{obj}:
fval(0483) = 2.2266E-03
rel. contribution = 0.0011 %

Fig. S0469 (AIOMFAC_output_1004)

H_2O (1) + 2,4-Dihydroxybenzaldehyde (2) + NaCl (3)

Temperature: 298 K

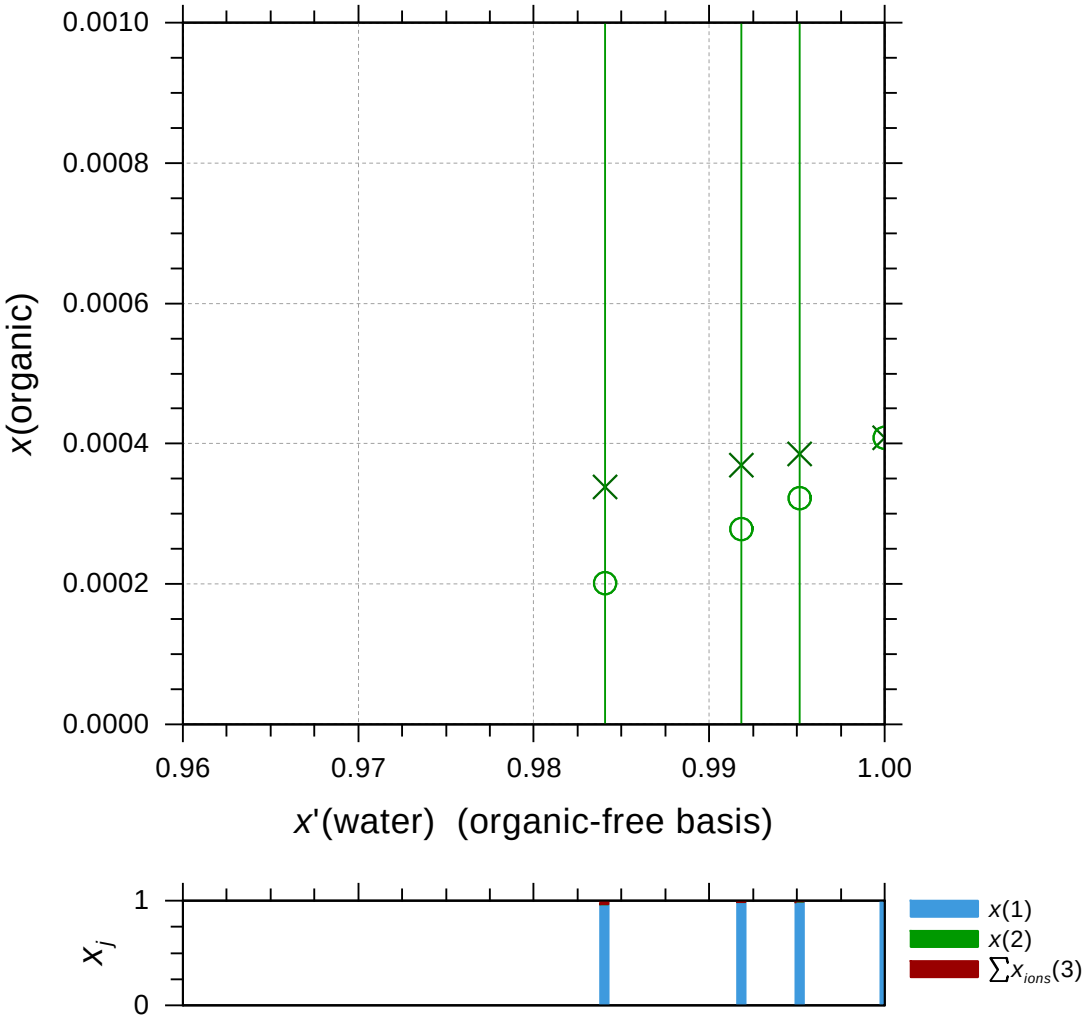


initial weighting of dataset:
$w^{init}(1004)$ = 1.000
dataset contribution to F_{obj}:
fval(1004) = 7.5005E-03
rel. contribution = 0.0036 %

Fig. S0470 (AIOMFAC_output_0466)

H_2O (1) + Benzene (2) + $NaNO_3$ (3)

Temperature: 298 K

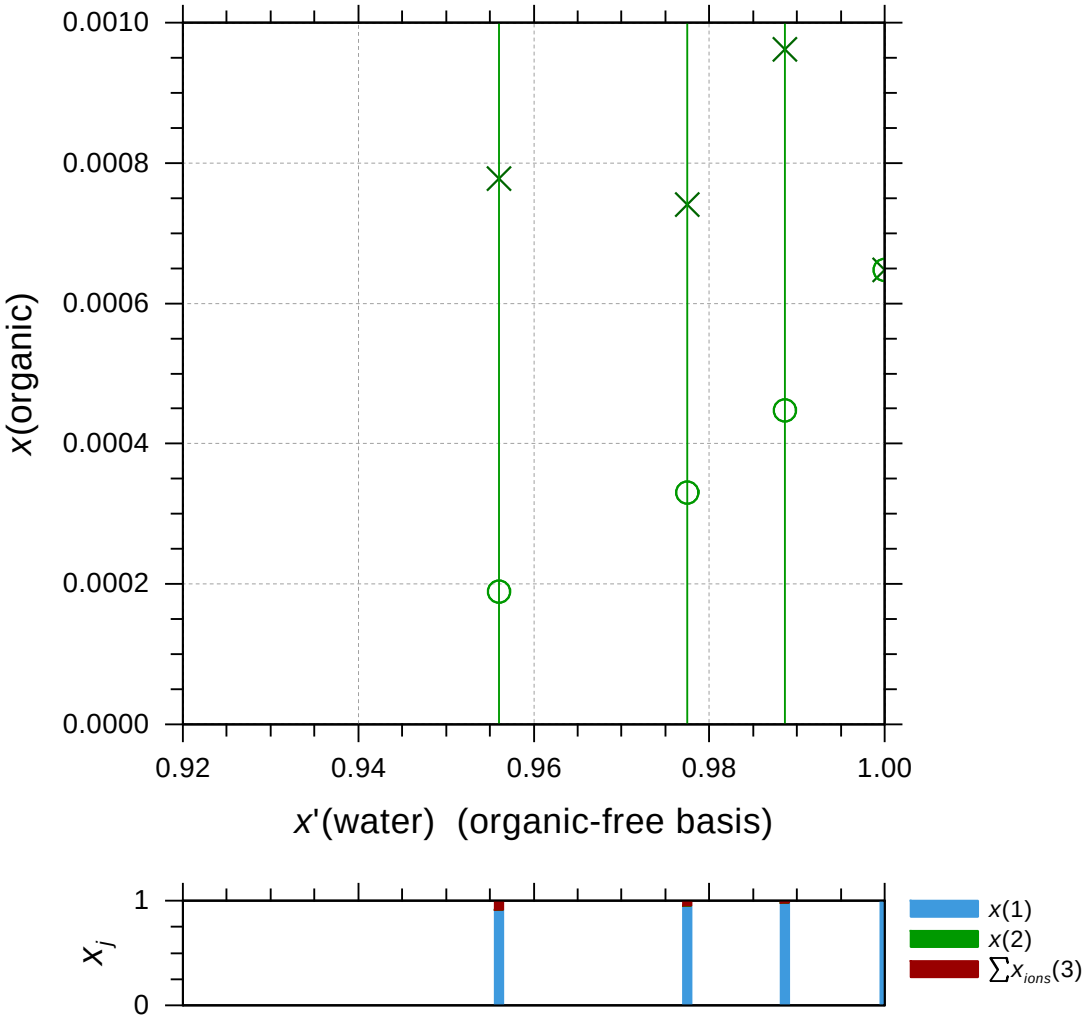


initial weighting of dataset:
$w^{init}(0466)$ = 1.000
dataset contribution to F_{obj}:
fval(0466) = 2.9067E-04
rel. contribution = 0.0001 %

Fig. S0471 (AIOMFAC_output_1003)

H_2O (1) + 2,4-Dihydroxybenzaldehyde (2) + NH_4Br (3)

Temperature: 298 K



initial weighting of dataset:

$w^{init}(1003)$ = 1.000

dataset contribution to F_{obj}:

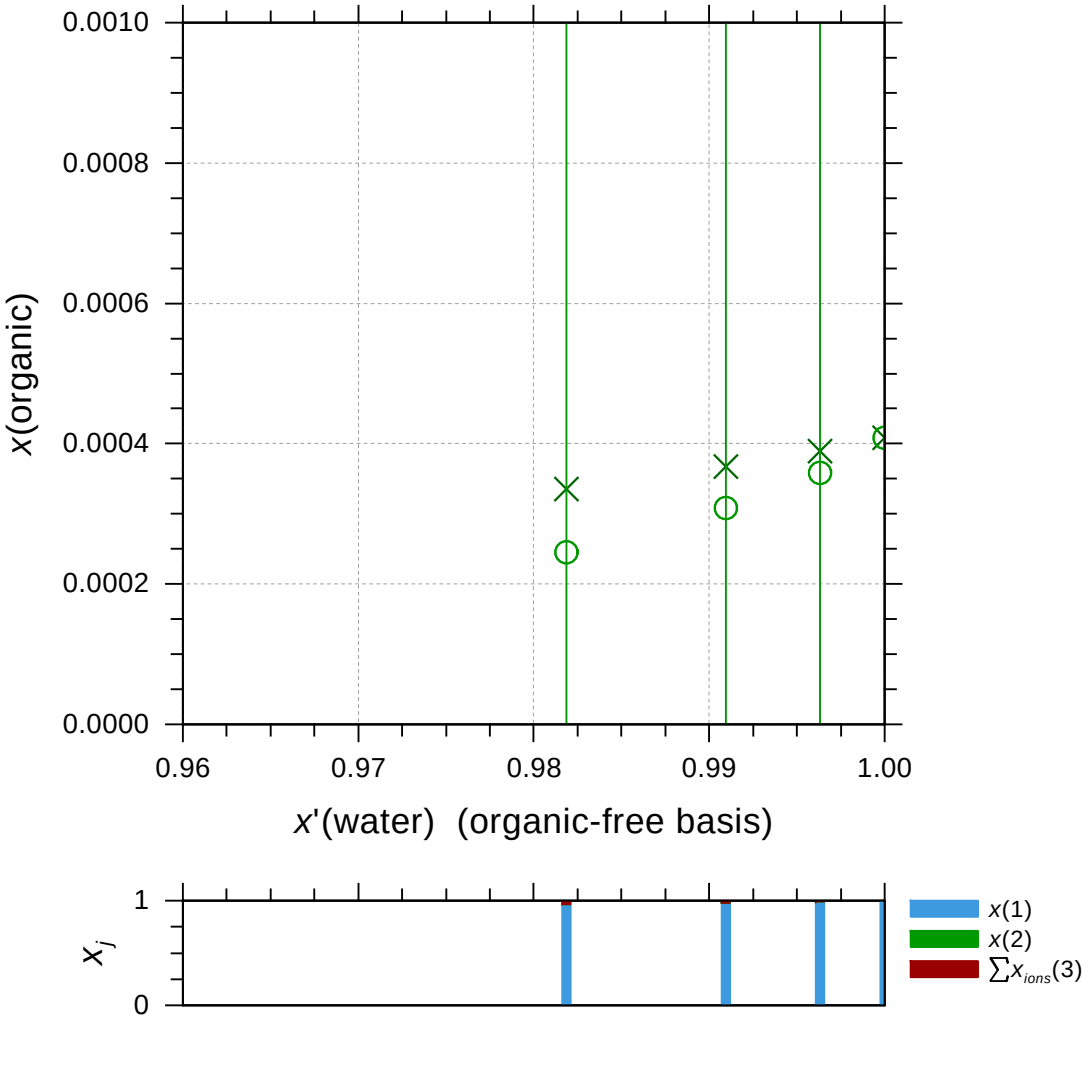
fval(1003) = 6.6436E-03

rel. contribution = 0.0032 %

Fig. S0472 (AIOMFAC_output_0470)

H_2O (1) + Benzene (2) + NH_4Cl (3)

Temperature: 298 K



initial weighting of dataset:
$w^{init}(0470)$ = 1.000
dataset contribution to F_{obj}:
fval(0470) = 1.1760E-04
rel. contribution = 0.0001 %